LEHIGH UNIVERSITY

DEVELOPMENT OF COMPUTER PROGRAM
FOR FIRE SUPPRESSANT FLUID FLOW

ANNUAL TECHNICAL REPORT, 1998

by

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Duke Engineering and Services, Inc.

December 1, 1998

19991202 024

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 074-0188

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188), Washington, DC 20503

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE December 1, 1998	3. REPORT TYPE AND DATES COVERED Annual Technical Report

4. TITLE AND SUBTITLE
Development of Computer Program for Fire Suppressant Fluid Flow

5. FUNDING NUMBERS
N/A

6. AUTHOR(S)
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Lehigh University   Duke Engineering and Services, Inc.
Institute of Thermo-Fluid Engineering &
Science
Bethlehem, PA 18015

8. PERFORMING ORGANIZATION REPORT NUMBER
N/A

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
SERDP
901 North Stuart St. Suite 303
Arlington, VA 22203

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
N/A

11. SUPPLEMENTARY NOTES
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12a. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for public release: distribution is unlimited.

12b. DISTRIBUTION CODE
A

13. ABSTRACT *(Maximum 200 Words)*

The objective of the project is to develop a computer code capable of predicting single- and two-phase hydrodynamic behavior of fire suppressant fluids during transport through piping systems. This new code will be able to predict pressure losses and flow rates for a wide variety of fluids, through piping systems with various combinations of fittings, over a broad range of pressure and composition conditions. The code will also be able to predict transient behavior for start and stop of flows, as well as for time varying pressure heads.

A key technical approach in the present program is utilization of advancements made in other applications that deal with multi-phase flows. In particular, the highly sophisticated computer codes that have been developed for thermal-hydraulic analysis of nuclear power systems have all the characteristics required for analysis of fire suppressant systems. Several relevant codes were reviewed and RELAP5 (MOD3, Version 3.2) was selected as the base code for the present work.

14. SUBJECT TERMS
SERDP, computer, program, suppressant, flow, hydrodynamic, fire, RELAP5

15. NUMBER OF PAGES
32

16. PRICE CODE
N/A

17. SECURITY CLASSIFICATION OF REPORT unclass	18. SECURITY CLASSIFICATION OF THIS PAGE unclass	19. SECURITY CLASSIFICATION OF ABSTRACT unclass	20. LIMITATION OF ABSTRACT UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102

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DEC 1998

ACKNOWLEDGEMENT

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SUMMARY

The objective of the project is to develop a computer code capable of predicting single- and two-phase hydrodynamic behavior of fire suppressant fluids during transport through piping systems. This new code will be able to predict pressure losses and flow rates for a wide variety of fluids, through piping systems with various combinations of fittings, over a broad range of pressure and composition conditions. The code will also be able to predict transient behavior for start and stop of flows, as well as for time varying pressure heads.

A key technical approach in the present program is utilization of advancements made in other applications that deal with multi-phase flows. In particular, the highly sophisticated computer codes that have been developed for thermal-hydraulic analysis of nuclear power systems have all the characteristics required for analysis of fire suppressant systems. These include models that account for relative slip between liquid and vapor phases, thermodynamic non-equilibrium between the phases, changes in two-phase flow regimes, critical choke flows, and transport of non-condensible gases. Such codes are also structured for numerical analysis of fast transients, well capable of the transients anticipated for suppressant systems. Several relevant codes were reviewed and RELAP5 (MOD3, Version 3.2) was selected as the base code for the present work.

The expected results from this project are:

a.   Collection of experimental data with candidate fire suppressants (both assembled from prior publications and new data from additional experiments),
b.   A product computer code, capable of calculating transient single and two-phase flows in piping systems for suppressant discharge.
This product code will represent state-of-art in the technology of two-phase flows. The code will be useful for analysis of suppressant systems with alternate suppressant fluids, and for engineering design of new fire suppressant systems.

This project was initiated in April, 1998. In this first year, progress has been as expected. The experimental test loop was fabricated and assembled. Selection of the base code was completed. The algorithm in the code for physical properties was evaluated to enable modifications to fluids other than water. As an example for suppressant fluids, the properties of Halon were obtained in a suitable form and incorporated into the code. A sample case for a fire suppression discharge was successfully completed.

NOMENCLATURE

A	Area
B_x	Gravitational acceleration in flow direction
C	Virtual mass coefficient
DISS	Dissipation term
FIF	Interfacial friction coefficient, liquid side
FIG	Interfacial friction coefficient, vapor side
FWF	Wall friction coefficient, liquid side
FWG	Wall friction coefficient, vapor side
M_s	Vapor mass
P	Pressure
Q_w	Wall heat transfer
Q_i	Interfacial heat transfer
Q_{gf}	Sensible heat transfer in presence of noncondensable
T	Temperature
U	Internal energy
V	Volume
X_n	Noncondensable quality
c_p	Specific heat at constant pressure
k	conductivity
s	entropy
t	time
v	velocity
x	distance

Greek Symbols

Γ	Mass generation per unit volume
α	Volume fraction
β	Isobaric thermal expansion coefficient
κ	Isothermal compressibility
μ	Dynamic viscosity
ρ	Density
ρ_m	Mixture density
σ	Surface tension
υ	Specific volume

Subscripts

I	Interface
g	vapor or gas
f	liquid
i	initial
sat	saturation

FIGRUE CAPTIONS

1. DESCRIPTION OF PROJECT AND OBJECTIVES

The objective is to develop a computer program (or code) capable of predicting the delivery rates of a fire suppressant fluid to a designated location, via a piping network system. The fluid will be a replacement to the currently widely used Halon.

The current delivery systems for Halon generally consist of a suppressant vessel connected to the delivery location by a piping network. The suppressant vessel is pressurized by an inert gas, usually nitrogen. The suppressant fluid is maintained in a liquid state by the pressurization of the system, usually up to several MPa. The system is activated by a quick opening valve in response to either an automatic or manual trigger. This causes the gas driver to expel the suppressant fluid through the piping system. The delivery system has to be able to begin delivering the fluid to the discharge location very quickly, generally within a few seconds. Complete discharge of the system is required to occur within 0.1 to 10 seconds.

Since Halon and its potential replacement fluids are in a vapor state at standard pressure and temperature, at the discharge location the fluid would be a two-phase mixture of superheated liquid and vapor. Thus significant thermodynamic and thermal non-equilibrium can be expected between the phases. Also, due to the large pressure difference between upstream source vessel and downstream exit, continuous flashing is anticipated as the fluid travels through the piping, and two-phase critical (choked) flow can occur at various locations.

Hence, to accurately predict performance of the delivery system, the computer code should be a transient two-phase code which allows for phase non-equilibrium. The short delivery times suggest fairly high flow rates, which promote homogeneous two-phase flow, i.e. little slip. However, in imbalanced piping networks, with side tees and other fittings, some separated flow could occur (stratified flows, slug/plug flow, etc.). Hence the code should be able to predict slip between phases and the corresponding effect on pressure drop. This can be especially important if separated flow encounters directional change, such as at a side tee. The ability to predict the transport of non-condensible gas is also important. The fluid, pressurized with a driver gas, is initially saturated with the gas. During the delivery, as the system depressurizes, the driver gas comes out of solution and expands. This gas evolution phenomenon needs to be accounted for. One additional requirement is that the code should be useful for estimation of the transient hydrodynamic loads in the piping network. Thus the momentum equations need to be sufficiently detailed to estimate the unbalanced force in piping sections between locations of elbows and other fittings.

There has been some work conducted on modeling Halon 1301 flows. In a 1988 summary of the state-of-the-art, DiNenno and Budnick (1988) indicate that most of the flow calculations are performed by vendors using proprietary methods. These methods are verified against standard NFPA procedures for calculations and by discharge to testing in sealed tests. However, there are significant uncertainties in the calculations and also in extrapolation of test results to actual configurations.

Therefore, the objective of the present work is to develop a computer code capable of predicting single and two-phase hydrodynamic behavior of fire suppressant fluids during transport through delivery piping systems.

A key technical approach in the present program is utilization of advancements made in other applications that deal with multi-phase flows. In particular, the highly sophisticated computer codes that have been developed for thermal-hydraulic analysis of nuclear power systems have all the characteristics required for analysis of fire suppressant systems. These include models that account for relative slip between liquid and vapor phases, thermodynamic non-equilibrium between the phases, changes in two-phase flow regimes, critical choke flows, and transport of non-condensible gases. Such codes are also structured for numerical analysis of fast transients, well capable of the transients anticipated for suppressant systems.

Furthermore, since the fluids being considered for use in fire suppressant systems is different from the water/steam system of nuclear power systems, physical property packages need to be modified and expanded. Here again, we are leveraging existing technology by borrowing from existing property packages. Specifically the REFPROP package, developed by the National Institute of Science and Technology (NIST), covers many refrigerant fluids including those that are potential candidates for the fire suppressant systems. We are complementing these property packages with additions to cover other suppressant candidates as required.

The present project contains an experimental task, to obtain data needed to assess the code. The experimental program envisions a discharge loop using new fire suppressants. In this experimental program, we are attempting to measure major flow parameters which have not been measured heretofore. These include measurements of instantaneous discharge flow rate and void fraction at various locations along the discharge pipe.

This program is being carried out as a team effort; the Institute of Thermo-Fluid Engineering and Science at Lehigh University is the main contractor. Duke Engineering and Services is subcontractor to Lehigh University and responsible for code development work.

The present report describes activities and accomplishments in the program during April-September 1998, and covers the following areas:
- Previous works and selection of the base code,
- Experimental work
- Code development activities,
- Plans for the next year.

2.   PREVIOUS WORKS AND SELECTION OF THE BASE CODE

2.1   Experimental Data with Fire Suppressants

To fully test the computer code developed in this research, comparisons of code predictions against experimental data will be made. A literature survey has been conducted to find possible sources for experimental data for transient two-phase flows. One widely referenced study is the "The Marviken Tests" conducted using water/steam for the nuclear reactor industry, Marviken Power Station (1982). These tests used a liquid/vapor filled vessel under high pressure and measured the vertical discharge characteristics as this system was released to atmospheric conditions. A similar test was carried out by Edwards and O'Brien (1979), but focused on the effects of a horizontal discharge. Even though the Marviken and Edwards tests were conducted with water/steam systems, they still provide some means for assessing portions of the code which use mechanistic models for predicting non-homogeneous, non-equilibrium two-phase flows. These mechanistic models are fluid-independent and are invoked for all fluids.

Three studies, which more closely reflect the intentions of the current study, have used fire suppressants as their test fluids, rather than water and steam. The work undertaken by Elliot et al. in 1984, include both theoretical and experimental investigations. In this work, Halon 1301 (widely used in both military and commercial applications) was used as the suppressant fluid. The tests discharged Halon under nitrogen gas pre-pressure, resulting in flow of a liquid/vapor/non-condensable-gas mixture through a configuration of piping and an end nozzle. This study provides data on pressure decay as a function of time, allowing for the estimation of discharge flow rates, which are useful for accessing code predictions. This study also provides observations of experimental phenomena as the discharge proceeded. An example is the phenomenon of evolution of the dissolved nitrogen from the liquid Halon, which causes an increase in the pressure of the discharge vessel and an increase in the driving force propelling the discharge of the fluid.

The most comprehensive tests conducted to this date were launched in the mid 1990's by the National Institute of Standards and Technology, Pitts et al. (1994) and Yang et al. (1995). Their tests not only utilized Halon 1301 as a test fluid, but also utilized HFC-125, HFC-227ea, and CF3I. They conducted several experimental runs with each fluid, providing extensive data for various pipe configurations and operating conditions. Experiments with different initial fill volumes, pressures, and temperatures were performed to determine their effects on the two-phase system. Their findings provide important information about the characteristics of the two-phase transient flow as it discharges from the source vessel and through the piping. The pressure histograms from this earlier program will be used as a benchmark in gauging the effectiveness of the code being developed in the current program.

These prior studies provide the beginning of an experimental database. However, there are no data on several key parameters important to code assessment. Primary among these is the instantaneous mass discharge rate and void fraction, at the exit of the source vessel and at the exit of the distribution pipe. Such parameters reflect the mechanisms of phase change (vaporization) and interfacial momentum transfer (slip velocity) that must be correctly modeled in the computer code. Without specific experimental measurements of such key parameters, it is

impossible to fully assess the validity of any prediction. This is the reason why the experimental program at Lehigh has been structured to obtain a number of additional measurements, above and beyond the usual measurement of pressure decay.

2.2   Physical Property Data for Fire Suppressant Fluids

Two-phase flow calculations require thermodynamic and transport properties of the fluid. These properties are required for single-phase liquid, for single-phase vapor, and for saturated vapor/liquid mixtures. The following thermodynamic properties are needed as functions of absolute pressure:

- Saturation temperature
- Specific heat for gas and liquid phases
- Thermal expansion coefficient for gas and liquid phases
- Isothermal compressibility for gas and liquid phases
- Specific volume for gas and liquid phases
- Specific entropy for gas and liquid phases

In addition, the following transport properties are also required for two-phase flow calculations:
- Dynamic viscosity for gas and liquid phases
- Thermal conductivity for gas and liquid phases
- Surface tension

Most fire suppressants are also used as refrigerants. The refrigerant property package REFPROP developed at NIST by Gallager et al. (1993) covers most of the fire suppressants. For example, it contains properties of Halon 1301, and present fire suppressant candidate FC-227ea. After evaluation, we find that REFPROP is a suitable package for determining the properties required by the new code for two-phase flow calculations with suppressant fluids.

2.3   Desired Feature of the New Code

As discussed in the original proposal, Chen, Tuzla, Sundaram (1997), the base code should be developed with some specific features in terms of its technical ability to model the basic phenomena of two-phase flows. In addition, user convenience and ease of development are also desirable features. The present development seeks to build the following features into the new code:

Required Features

1.   Non-homogeneous two-phase flow accounting for relative slip between phases
2.   Non-equilibrium two-phase flow, allowing for metastable conditions during flashing
3.   Choking under single and two-phase conditions
4.   Non-condensibles (dissolved gas) transport
5.   Multi-component mixtures (liquids, gases, powders)
6.   Flexible system modeling capability (choice of piping components and layout)

7. Robust set of equations, for simulation of fast transient two-phase flows (for example, momentum equation to include frictional losses, energy equation to include dissipation)
8. Demonstrated ability to model representative systems (assessment against experiments)

Desirable Features

1. Non-proprietary, publicly available
2. Portable to various computer and operating systems
3. Ease of development (well-documented, flexible architecture)
4. Ease of application (user-friendly inputs)

There are other intangible features that have also been considered, such as the existence of an active user group, which would facilitate future modifications and developments.

2.4   Two-Phase Codes Considered for this Work

The relevant codes are those used in the nuclear industry for loss-of-coolant accident analyses (LOCA). These codes address the major phenomena of interest (non-homogeneous, non-equilibrium two-phase flows, choking conditions, fast transients). The survey was limited to codes developed and available in the United States and consisted of RELAP5, RETRAN, TRAC-P, TRAC-B and GOTHIC. Codes developed in other countries that could be used (ATHLET, CATHARE) were not considered because easy access to these codes may not be available.

All these codes have many of the required and desirable features for the present application. They are all based on a two-fluid model of two-phase flow, with constitutive equations to specify the interfacial transport terms. Although some of them have multi-dimensional modeling capability, they are predominantly used in a one-dimensional mode. A brief history of these codes is presented below, with some relevant information:

1. RELAP5

The latest version of this code is RELAP5/MOD3, version 3.2, available since 1995, RELAP5/MOD3 Code Manual (1995). This code was developed at the Idaho National Engineering and Environmental Laboratories (INEEL) under sponsorship of the U.S. Nuclear Regulatory Commission (USNRC). It is used for a variety of reactor accident analyses, including LOCA analyses, for a variety of types of reactors. It is also used in a variety of general thermal-hydraulic analyses in nuclear and non-nuclear systems. It is non-proprietary, and is publicly available, for a transmittal fee, from the USNRC. An active user group, including U.S. and international organizations, meets once a year. Information on user problems, error correction, etc. are transmitted to user group members once every three months.

2. RETRAN

The latest version of this code is RETRAN-03, RETRAN-03 (1992). This code was developed by Computer Simulations and Analysis, Inc., under sponsorship of the Electric Power Research Institute (EPRI). It is used primarily for analyses of reactor systems, with focus on the primary

cooling system, and usually for non-LOCA scenarios. It is proprietary, and can be obtained from EPRI, with license fees and user group membership fees. The user group, including U.S. and international organizations, is active and meets regularly.

3. TRAC-P

The latest version of this code is TRAC-PF1/MOD2, TRAC-PF1/MOD2 Code (1992). It was developed by the Los Alamos National Laboratory (LANL) under USNRC sponsorship. It is used primarily for LOCA analysis of pressurized water reactors. It is non-proprietary and can be obtained, for a transmittal fee, from the USNRC. There are relatively small number of users and no regular user group meetings.

4. TRAC-B

The latest version of this code is TRAC-BF1/MOD1, TRAC-BF1/MOD1 Code (1992) and TRAC-BF1/MOD1 Models (1992). It was developed by INEL under USNRC sponsorship. It is used for accident analyses of boiling water reactors. It is non-proprietary and can be obtained from the USNRC for a transmittal fee. The user group is active and meets regularly.

5. GOTHIC

The latest version of this code is GOTHIC version 5.0, GOTHIC Containment Analysis Package Version 5.0 (1995). It was developed by Numerical Applications, Inc., under EPRI sponsorship. It is used primarily for analysis of reactor containments. It was developed from the COBRA series of codes originally developed at the Pacific Northwest Laboratory under USNRC sponsorship. The original COBRA series of codes are non-proprietary, but were not maintained by the USNRC after the mid-1980's, and are now difficult to obtain. The GOTHIC code is proprietary and can be obtained from EPRI for license fees and user membership fees. The user group is active and meets regularly.

2.5   Selection of the Base Code

The documentation for each of the candidate codes were reviewed. It was concluded that all the codes listed above have many of the required and desirable features, but none have all the features. The conclusion was that the RELAP5 code (MOD3, version 3.2) has more of the required and desirable features than the other codes. In addition, the code has been adapted previously for operation with a fluid other than water, and the code architecture to accomplish this is available in the latest version of the code. This is especially helpful for insertion of new property packages for suppressant fluids. Besides, the code development team at Duke Engineering and Services has accumulated significant operating experience with RELAP5, thus providing confidence that the program objectives could be met successfully with this code. Based on these characteristics, RELAP5/MOD3 version 3.2 has been selected as the base code platform for the present development.

3. EXPERIMENTAL WORK

The objective for the experimental work is to collect experimental data using new fire suppressant agents as test fluids. This data will then be used in the assessment of the product code for simulating possible suppressant delivery systems. Descriptions of pertinent dimensions and design features of the test facility are provided below.

3.1 Experimental Test Facility

The test facility consists of a source vessel for the suppressant fluid, a quick opening discharge valve, a holding rack, a piping network, and a collection tank. This arrangement allows the system to be operated as closed loop, with recycle of the test fluid. A simple schematic has been provided in figure 3.1, showing the layout of the facility. The dimensions of this test system adhere as closely as possible to the standard sizes used in present-day fire suppression systems.

The source vessel, one of the main components of the facility, is shown schematically in Figure 3.2. The source vessel has a total internal volume of 3.81 liters and will initially be charged with liquid to about 60% of that volume. The source vessel was constructed from a 2 meter long piece of 2 inch (5.08 cm) nominal diameter stainless steel pipe with an internal diameter of 1.94 inches (4.93 cm) and a wall thickness of 0.22 inches (0.55 cm). Using a vessel of large length-diameter ratio improves the accuracy of measuring liquid inventory. This will be explained in more detail in Section 3.3, but simply speaking, we will use a pressure difference associated with the static head of the liquid in the vessel to measure the liquid inventory in the vessel at any time during the experimental run. The long length, or height, of the source vessel provides a greater range of static head measurements, thus increasing the accuracy of determining transient liquid inventory. This pipe will be positioned vertically and capped at both ends by stainless steel pipe flanges approximately 1 inch (2.54 cm) thick. Two slip-on flanges with o-ring grooves for the pressure seals were welded to either end of the pipe so that the top and bottom plates could be bolted in place. The top plate has an identical outer diameter as the flanges, at 6.5 inches (16.51 cm), and was tapped to allow for a mixing line inlet and a fill/relief line. The bottom plate has a larger diameter of 11 inches (27.94 cm) for the purpose of anchoring the vessel to the holding rack. This plate has also been tapped to allow the discharge valve to be screwed into place and sealed with a crushable, tempered aluminum gasket. Other features incorporated into the source vessel include pressure and temperature ports, a liquid level gauge, a mixing line, and the differential pressure transducer with silicon fluid transmission line for measurement of liquid inventory.

Since tests will require pressures up to 40-50 atmospheres in the source vessel, pressurization by a nitrogen cover gas will be employed. As shown in figure 3.3, for FC-227ea, the equilibrium vapor pressure of suppressant fluids will only reach about 5 atmospheres at room temperature, insufficient for the desired pressure without the additional partial pressure of an inert cover gas such as nitrogen. A potential problem with this method is that the total pressure in the vessel will not reach equilibrium until the liquid has become saturated with dissolved nitrogen. In order to expedite this process, a mixing system has been incorporated into the design, using a pump to

recycle liquid suppressant from the bottom of the source vessel to a spray nozzle located in the vapor/gas space. By spraying small droplets of liquid through the nitrogen gas, the surface area of liquid in contact with nitrogen will increase, therefore increasing the rate at which nitrogen can be dissolved into the liquid.

Additional ports in the source vessel include an opening near the top, which will serve as the connection to nitrogen supply and as one leg of the transmission line for the differential pressure transducer. A liquid level gauge made of armored glass has also been attached to the middle section of the vessel to visually determine the liquid fill level in the vessel at the beginning of each experimental run. Also, there are two thermocouple ports for the vapor and liquid spaces and a pressure port in the vapor space. The last port is in the top plate, providing access for filling of the vessel and also serving as a connection for a safety pressure-relief device.

The next pertinent item in our design is the release mechanism of the source vessel, for initiating discharge of the test agent. A quick-opening plunger valve with an inlet diameter of 1.25 inches (3.18 cm) and an exit diameter of 1.75 inches (4.45 cm) is used for this purpose. This valve, shown in figure 3.4, is a Model MV121KJ-2 valve made by Marotta Scientific Controls Inc. A feature of this valve is the use of the fluid pressure to drive the plunger upon command, thereby eliminating the need for springs or motors. To set or close the valve, the plunger is pushed up into its armed position and held in place by a small locking latch. Two O-rings are attached to the plunger to form a pressure seal along the valve casing. Pressure must then be provided on the inlet side of the valve for the valve to operate properly. To open the valve, an electrical charge provided by 20-volt DC power source releases the latch, allowing the fluid pressure to rapidly drive open the plunger. This release is much faster than that of traditional solenoid valves, and is similar to that of a burst diaphragm or explosive-charge release, which is used in present-day suppression systems. The valve is connected to the 1/2-inch discharge piping in the loop by a tapered transition piece. This transition incorporates a flange connection to permit access to the O-ring seals on the plunger for lubrication.

The piping in the test facility consists of 1/2-inch nominal diameter stainless steel pipe with an internal diameter of 0.546 inches (1.39 cm) and a wall thickness of 0.15 inches (0.38 cm). There are five other pieces including the adapter piece described above, which make up the discharge piping system. Two of these pieces are approximately 12 inches (30.5 cm) in length with flanges at either end to provide for easy disassembly. All the flanges are machined with an O-ring groove to provide an adequate seal against the high pressures experienced in the tests. These 12-inch sections will be used as access points at the beginning and end of the piping system, as indicated in figure 3.5. They will also be the first and last locations of the pressure and temperature measurement ports. Ports for the pressure transducers and film thermocouples used for these measurements required special weld fittings in order to insure a complete pressure seal in the loop. These fitting were specially designed to cause minimal disturbance to the flow, while allowing for the sensor to be as close to the flow as possible. See figure 3.6 for a schematic diagram of these fittings.

The other two pieces in the piping system include a composite pipe section used for the void fraction measurement and a long middle section of pipe. The composite section and its role in measurement of void fractions will be described in section 3.5. The long middle section of

pipe represents the distribution spool piece often found in fire-suppressant piping systems. Both ends are flanged and are capped by valves, allowing for the isolation of this section. The middle piece will be tapped in the middle for temperature and pressure ports as described previously. This middle piece of long discharge piping allows for easy reconfiguration to different piping schemes in the future (i.e. inclusion of tees or elbows). This whole piping system is then connected by a flange to the collection vessel, providing a closed flow path from the source vessel, through the piping system, to the collection vessel.

The collection vessel is designed to serve two purposes: to catch the test fluid for recycle and to enable monitoring of the transient discharge pressure during test runs. The collection vessel has an internal volume of approximately 30 liters, chosen to limit the final pressure after discharge to less than 8-10 atmospheres. This vessel is made of a 10 inches diameter stainless steel pipe with an internal diameter of 9.56 inches (24.3 cm) and a wall thickness of 0.59 inches (1.50 cm). The bottom of the collection vessel is a hemispheric cap with a 1/2-inch port, to be used for emptying the contents. At the top end is a pair of 1.75 inches thick flanges sealed by an O-ring. The outside flange has access holes to allow for a cooling coil, a vacuum line, and a temperature port. The cooling coil will carry either cold water or liquid nitrogen, for the purpose of recondensing the spent suppressant fluid for recycle. Additional ports in the sides of the vessel provide connections for the piping system and a fast-response pressure transducer.

In anticipation of potentially large reaction forces during fluid discharge, a rugged framework was designed to support the test facility. As shown in Fig. 3.7, an 8 inch I-beam, 10 feet high, was chosen to give a rigid backing for the source vessel while being heavy enough to dampen any vibrations exhibited during the test runs. This rack I-beam is directly bolted to the building structure for rigidity. The rack I-beam has three welded shelves for use in supporting the source vessel. The first is positioned just below the middle of the beam and is used to hold the source vessel from the bottom. Since this area experiences most of the forces during the discharge tests, the shelf in this area is bolted to the large flange at the bottom of the source vessel. This shelf is equipped with support legs for added stability. The next shelf is located near the top of the rack and anchors the top section of the source vessel by clamping to the 2-inch pipe. The last shelf, positioned lower down on the beam, is used to hold the mixing pump. The I-beam is also equipped with boltholes along its face in order to add support structures for the level gauges and mixing lines. As for the piping system, it is supported by a metal framework, which has provisions for clamping the pipe and preventing movement in both horizontal and vertical directions. The collection vessel is attached to a movable dolly to allow for opening of the piping system when access is necessary. To account for substantial forces associated with the fluid discharging into the vessel, the collection vessel is held in place by support braces attached to a building I-beam.

The fabrication of the test loop is close to completion, with pressure testing and trial test runs expected to start in December 1998.

3.2 Pressure Sensors

The test facility is equipped to measure instantaneous pressure readings in the source vessel, along the piping system, and in the collection vessel by means of fast response pressure

transducers. The pressure transducers are Entran Model EPX-V01 with a range of 0-1000 PSIG (0-68 atmospheres). These transducers have a diaphragm which deflects according to the difference of the pressures experienced at its front and back sides and provides an output through a strain gauge bridge located on the back side of the diaphragm. In order to install these transducers at measurement locations, special fittings had to be designed and fabricated. As explained previously in section 3.1, it is desirable to locate the transducers as flush to the inside surface of the pipe as possible, in order to minimize disturbances to the flow. This was accomplished with the specially designed fittings shown in figure 3.6. With this fitting welded into place on the pipe, the transducer can be screwed into the tapped hole, allowing an O-ring to seal against the high fluid pressures.

To test the response time of the transducers in the operating pressure range, a bench top experiment was conducted. The transducer was screwed into a small chamber, which was connected to a compressed nitrogen line and a 1/2-inch-venting valve. The chamber was rapidly pressurized to about 30 atmospheres by opening the compressed gas line, while the back of the transducer remained exposed to atmospheric pressure. The supply line was next closed and the pressure was then quickly vented to atmosphere by opening the vent valve. The output of the pressure transducer was recorded with a data acquisition system at a 1000 Hz frequency. The transient pressure signals, for both the pressurization and depressurization, are shown in figures 3.8-3.10. Figure 3.8 shows the entire test sequence, where the transducer was initially exposed to atmospheric pressure, then the chamber was pressurized, and finally rapidly depressurized. Figure 3.9 shows an enlargement of the pressurization record; notice that the entire pressurization change was sensed by the transducer in less than 150 milliseconds. Figure 3.10 shows an enlargement of the depressurization record; notice that the depressurization transient was sensed by the transducer in less than 200 milliseconds. These two figures show that the response time of the transducers is only a few milliseconds and is acceptable for the present application.

3.3 Flow Rate Sensor

As mentioned above, a key parameter that we wish to measure is the instantaneous mass flow rate of fluid during transient discharge from the source vessel. To best of our knowledge, this has not been successfully measured in prior experiments due to its inherent difficulty. If fluid inventory in the source vessel could be measured as a function of time, then the rate of discharge would be given by the gradient of inventory versus time. Because of possible void generation in the liquid (due to gas evolution) and associated level swelling, observation of liquid level does not provide indication of fluid inventory. Our approach is to measure the static head of fluid in the source vessel, as a dynamic function of time. Since frictional and kinetic terms are negligible in the overall momentum balance for conditions in the vessel, we expect to obtain the fluid inventory in the vessel directly from static head measurements:

$$M = \frac{A}{g} \bullet \Delta P \qquad (3.3-1)$$

where M is the fluid inventory, A is the cross-sectional area of the vessel, g is gravitational acceleration, and ΔP is the pressure difference from bottom to top of vessel (the static head). The instantaneous rate of mass flow out of the vessel is then obtained from the time derivative,

$$\dot{m} = \frac{dM}{dt} = \frac{A}{g} \bullet \frac{d\Delta P}{dt} m \qquad (3.3\text{-}2)$$

To obtain desired accuracy for rate of mass flow, precise measurement of ΔP is necessary. We intend to use a differential pressure transducer to obtain this static head ΔP. As shown in figure 3.2, this transducer will be connected to the vapor space and the liquid volume at top and bottom of the source vessel, respectively. To maximize response time, the liquid connection is installed directly at the vessel wall (without transmission line). The vapor connection is a transmission line filled with inert silicon oil. Figure 3.11 shows a diagram of the set up for this differential pressure transducer, designed specifically for this application. With this arrangement, pressure signals will be transmitted to the transducer at speed of sound in liquid, sufficiently fast to obtain dynamic data during suppressant discharge.

We have purchased a differential pressure transducer for this measurement of the discharge flow rate. This differential transducer is similar to the gauge pressure transducer described above, with suitable change in the measurement range. A special bench experiment has been prepared to test the transducer for response time at anticipated run conditions. In the bench test, the differential pressure transducer will be subjected to rapid changes of ΔP and output signals recorded at high frequency. The measured response, at various levels of pressure difference, will provide evidence of the instrumentation's inherent time constant. These bench tests are currently in progress.

3.4   Temperature Measurement Sensors

Fluid temperatures along the discharge pipe are to be measured using film thermocouples. It has been experimentally shown at Lehigh, Cokmez-Tuzla, Tuzla, Chen (1993), that this type of thermocouple can provide response times in the order of milliseconds. A schematic of the film thermocouple is shown in Figure 3.12. Since the hot junction of the thermocouple is comprised of the metallic film, it is essential to maintain a continuos electric conductive-path through that film. Two issues are involved; compatibility of the film material to the test fluid, and the erosive effects of the flow on the film. During the past experiments at Lehigh, a metallo-organic paint was used to make the film at the tip of the thermocouple. This film worked well in experiments with high temperature steam and water. After a search for alternatives, we decided once again to use this same material for the junction film. A bench setup was prepared to test the thermocouple with this film junction. After forming the film, the thermocouple assembly was exposed to test liquids for duration of a minute. So far, tests with HFC-134a refrigerant indicate the junction film to hold up well to such exposure. However, tests with the actual suppressant to be used (FC-227ea) still need to be carried out. This effort has been delayed because of difficulty in acquiring FC-227ea fluid. No bench test for erosion will be attempted, due to the significant effort involved. We will fabricate the junction films as robustly as possible and trust to their durability in actual runs. Should erosion damage occur, it will be possible to remake the film junctions and reinstall the thermocouples.

3.5   Void Fraction Sensor

One of the major flow variables for two-phase flow is the void fraction. Many flow parameters, such as thermodynamic quality, vapor and liquid mass fluxes, and transport properties of vapor and liquid affect the void fraction. In turn, the void fraction strongly affects pressure drop, holdup inventory, and flow rate for any given operating condition. Thus, it is desirable to experimentally measure the void fraction during the transient discharge of suppressant. Once again, this is a difficult measurement in two-phase flows and were not attempted in prior experiments of suppressant flow. In the present work we are attempting to measure the transient void fraction at the discharge pipe. The desirable features of a sensor for void fraction are:

- No disturbance on flow
- Integrate the void fraction over the cross-section
- Fast response

Based on previous experience at Lehigh University, we selected to use a capacitance sensing method for this measurement, in expectation that this method will satisfy all of the above desirable features.

A number of different capacitance probes were designed, fabricated, and bench tested during this year. The final probe configuration is shown schematically in Fig. 3.13. As indicated the probe consists of a positive electrode and a ground electrode, both placed on the outside surface of the discharge pipe. The section of the discharge pipe at this location needs to be electrically nonconductive to allow capacitance measurements. For the purpose of these bench tests, a glass tube is being used as the pipe material. The positive electrode is a strip of copper in contact with the outer surface of the pipe. The electrode span is as wide as the ID of the pipe. The ground electrode is placed on the opposing side of the pipe. When powered by a high-frequency voltage, this probe would measure an overall capacitance between the two electrodes, which includes the whole cross-section of the tube. This capacitance can then be calibrated to give the void fraction of the vapor/liquid mixture in the pipe. There is a guard electrode around the positive electrode to prevent/reduce stray capacitance.

This probe was tested on a bench loop with water and HFC-134a. The schematic of the bench setup is shown in Fig. 3.14. The test started with the glass tube filled with water. During the test, the tube was emptied from the bottom so that the liquid level receded with a constant speed. The recorded signal from the capacitance sensor calculated void fraction are shown in Fig. 15a and b. It is seen that initially the probe senses 100% liquid in the tube. As the liquid level approaches the top of the sensor, the signal slowly starts to show some void in the sensing volume (edge effect). When the liquid level is within the sensing volume, the variation of measured void fraction is linear with liquid level. Again, there is an edge effect when the liquid level is close to the bottom edge of the sensing volume. Later, when the liquid level falls clear of the sensing volume, the probe senses all air in the tube. Despite the fact that we guard the sensing area, there are some edge effects in the axial direction. The above test was repeated with HFC-134a under pressure and similar results were observed. The dielectric constants of liquid

water, air, and liquid and vapor HFC-134a are provided in Table 3.5.1. It is seen that there is significant difference between the dielectric constants of liquid water and liquid HFC. Therefore, different size electrodes may be needed for each fluid. The edge effect observed are undesirable and modifications to the probe are in progress to reduce or eliminate it. Tests are in progress to eliminate the edge effects. Tests with FC-227ea will be carried out as soon as the fluid is acquired.

Table 3.5.1: Dielectric Constant of Selected Substances

Temperature (°C)	Water (Liquid)	Air (P=760 mmHg)	HFC-134a (Liquid)
0	87.69	1	-
10	83.82	-	-
20	80.08	-	9.22
25	78.25	-	-

Reference: Lide, David R., CRC Handbook, 7th Ed.

3.6   Trial Tests

Upon completion of fabrication of the test loop, check-out tests for the loop and instrumentation will be conducted using CO_2. CO_2 was chosen due to the fact that it is in the liquid state under a pressure of approximately 55 atmospheres and will vaporize as the pressure drops, similar to what happens to a fire suppressant. The primary objective of these CO_2 tests is to confirm our system design and verify performance of instrumentation. As a secondary objective, these data will provide another benchmark for comparison with predictions obtained from our new code.

4. CODE DEVELOPMENT WORK

4.1 Code Development Tasks

As discussed in Section 2, the base code is RELAP5/MOD3.2, hereafter referred to as RELAP5. The required and desirable features of the code needed for modeling fire suppressant fluid systems were also identified in Section 2. This section describes the development tasks needed to convert RELAP5 for the intended use. Section 4.1.1 presents a brief description of RELAP5, which forms the basis for the specific development tasks identified in Section 4.1.2.

4.1.1 Relap5 Description

RELAP5 (RELAP5-1, 1995) is a computer program (or computer code) that can be used to predict transient two-phase flows in piping networks and other fluid systems. It was developed primarily for nuclear plant transient and accident analyses, and therefore uses water as the working fluid. It is based on a one-dimensional, two-fluid model of two-phase flow and allows prediction of non-homogeneous, non-equilibrium conditions. It is written in Standard FORTRAN-90, and was originally developed to run on the UNIX Operating System, but has been adapted to other operating environments. The version of RELAP5 chosen for further development is generally considered to be machine-independent and portable to a variety of commonly used operating systems.

To run RELAP5, a user generates an input file. This input file is essentially the description of the problem to be executed. It contains the geometrical description of the system under analysis, the necessary boundary and initial conditions, and other constraints imposed by the user, such as partition of the system into control volumes (nodalization), selection of particular code options and control of the time step used in the numerical solution. The code documentation contains a user manual (RELAP5-2, 1995) describing how to generate an input file.

In executing the program, RELAP5 generates two files, an output file that can be read by the user, and a restart file written in binary format. The output file provides information requested by the user in the input file. The restart file contains all the information the code needs such that the user can restart the code to run for a longer time period, with or without additional changes to the problem description, and is also used for generating graphical output. This process of executing the code and managing the results is retained in this development process because it provides a great deal of flexibility and control to the user.

The code also contains many user-convenient features and special models, which were developed primarily for nuclear plant analyses, such as the definition of specific components in nuclear systems, and code models to capture the transient behavior of nuclear fuel rods. Some of these are useful for the intended application to fire suppressant fluids and fluid systems, and some are not. At this point in the development process, all the existing features of RELAP5 are retained, unless it becomes necessary to remove them.

The thermal-hydraulic model of RELAP5 solves eight field equations for eight primary variables as a function of time (t) and distance (x). The eight primary dependent variables are pressure (P),

phasic specific internal energies (U_g,U_f), vapor volume fraction or void fraction (α_g), phasic velocities (v_g,v_f), noncondensable quality (X_n), and boron density (ρ_b). Note that the noncondensable quality is defined as the mass fraction of noncondensables in the gas phase, the remaining fraction being the mass fraction of steam in the gas phase. The boron density is not relevant to our application and hence there are essentially seven field equations with seven primary dependent variables. Of these seven variables, five are state variables (P,U_g,U_f,α_g,X_n) and two are velocities (v_g,v_f). The corresponding seven field equations are the conservation equations for mass, momentum and energy for each phase, and the conservation of mass for the noncondensables. The equations are described in detail in RELAP5-1, 1995. The simple forms of these equations are shown below, as one-dimensional area-averaged equations, on a per unit volume basis.

Conservation of Mass:

Gas Phase:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_g \rho_g v_g A) = \Gamma_g \qquad (4.1\text{-}1)$$

Liquid Phase:

$$\frac{\partial}{\partial t}(\alpha_f \rho_f) + \frac{1}{A}\frac{\partial}{\partial x}(\alpha_f \rho_f v_f A) = \Gamma_f \qquad (4.1\text{-}2)$$

The term on the right hand side of equation 4.1-1 is the interfacial vapor generation per unit volume.

Conservation of Momentum:

Gas Phase:

$$\alpha_g \rho_g A \frac{\partial v_g}{\partial t} + \frac{1}{2}\alpha_g \rho_g A \frac{\partial v_g^2}{\partial x} = -\alpha_g A \frac{\partial P}{\partial x} + \alpha_g \rho_g B_x A - (\alpha_g \rho_g A)FWG(v_g)$$
$$+ \Gamma_g A(v_{gI} - v_g) - (\alpha_g \rho_g A)FIG(v_g - v_f) \qquad (4.1\text{-}3)$$
$$- C\alpha_g \alpha_f \rho_m A \left[\frac{\partial(v_g - v_f)}{\partial t} + v_f \frac{\partial v_g}{\partial x} - v_g \frac{\partial v_f}{\partial x} \right]$$

Liquid Phase:

$$\alpha_f \rho_f A \frac{\partial v_f}{\partial t} + \frac{1}{2} \alpha_f \rho_f A \frac{\partial v_f^2}{\partial x} = -\alpha_f A \frac{\partial P}{\partial x} + \alpha_f \rho_f B_x A - (\alpha_f \rho_f A) FWF(v_f)$$

$$+\Gamma_f A(v_{fi} - v_f) - (\alpha_f \rho_f A) FIF(v_f - v_g) \qquad (4.1-4)$$

$$-C\alpha_f \alpha_g \rho_m A \left[\frac{\partial(v_f - v_g)}{\partial t} + v_g \frac{\partial v_f}{\partial x} - v_f \frac{\partial v_g}{\partial x} \right]$$

On the right hand side of equation 4.1-3, the second term is the body force and the subsequent terms are the wall friction, momentum transfer due to mass transfer, interfacial frictional drag and force due to virtual mass.

Conservation of Thermal Energy:

Gas Phase:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g U_g) + \frac{1}{A} \frac{\partial}{\partial x}(\alpha_g \rho_g U_g v_g A) = -P \frac{\partial \alpha_g}{\partial t} - \frac{P}{A} \frac{\partial}{\partial x}(\alpha_g v_g A)$$

$$Q_{wg} + Q_{ig} + \Gamma_g h_g - Q_{gf} + DISS_g \qquad (4.1-5)$$

Liquid Phase:

$$\frac{\partial}{\partial t}(\alpha_f \rho_f U_f) + \frac{1}{A} \frac{\partial}{\partial x}(\alpha_f \rho_f U_f v_f A) = -P \frac{\partial \alpha_f}{\partial t} - \frac{P}{A} \frac{\partial}{\partial x}(\alpha_f v_f A)$$

$$Q_{wf} + Q_{if} + \Gamma_f h_f + Q_{gf} + DISS_f \qquad (4.1-6)$$

On the right hand side of equation 4.1-5, the third to last terms are the wall heat transfer, interfacial heat transfer, energy transfer due to mass transfer, sensible heat due to presence of noncondensables, and dissipation.

Conservation of Mass for Noncondensables:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g X_n) + \frac{1}{A} \frac{\partial}{\partial x}(\alpha_g \rho_g X_n v_g A) = 0 \qquad (4.1-7)$$

Note that this assumes that there is no generation of noncondensables. Thus this equation essentially conserves mass of noncondensables existing in the system, and allows transport/distribution of the noncondensables along with the gas phase. It is assumed that the noncondensables are transported at the same velocity as the steam in the gas phase, that they are in thermal equilibrium with the steam, and that the properties of the gas phase are mixture properties of the steam/noncondensable mixture. The sensible heat transfer terms due to the presence of noncondensables in the energy equations represent heat transfer at the noncondensable gas-liquid interface. This is necessary because the interfacial terms use saturation temperature based on the local steam partial pressure.

It is assumed that at the gas-liquid interface, there is no storage of mass, momentum or energy. Thus when equations 4.1-1 and 4.1-2 are summed, the right hand side becomes zero. Similarly, summing equations 4.1-3 and 4.1-4 provides a relationship between the interfacial drag terms FIG and FIF. And summing equations 4.1-4 and 4.1-5 provides a relationship between the interfacial mass transfer and interfacial heat transfer. These are the essentially the interface conditions needed for closure of the conservation equations.

To get closure for solution of the set of equations, several terms on the right hand side of the conservation equations need to be specified, such as FWG, FIG, Q_{wg} and Q_{ig}. These are the constitutive relations. Typically, these are based on mechanistic models and empirical correlations, and are written in terms of velocities, thermodynamic and transport properties, and the temperature of the liquid and gas phases. Thus, additional relationships have to be defined to relate these to the primary dependent variables of the code.

To solve the above set of equations, the differential conservation equations are cast into a numerically convenient set of finite difference equations, using a staggered spatial mesh arrangement. In this method, mass and energy are conserved over a control volume while momentum is conserved over a cell centered on the mass and energy cell boundaries. A semi-implicit method is followed for time advancement where the implicit terms are formulated to be linear in the dependent variables at the new time. Essentially, this requires specification of the partial derivatives of fluid density with respect to the primary dependent variables.

The governing equations, together with the interface conditions, constitutive relations, thermodynamic and transport properties, and property derivatives, as a function of the primary dependent variables, form a closed set of equations. RELAP5 solves this set for the primary dependent variables as a function of time and spatial location.

4.1.2 Development Tasks

The above discussion provides the basis for identifying specific development tasks needed to adapt RELAP5 for use with fire suppressant fluids and fluid systems. These are described below.

1. Incorporation of fluid properties and derivatives: This task is to replace the current water-steam thermodynamic and transport properties with those for a fire suppressant fluid. Since there are several fluids under consideration for replacing Halon 1301, the code needs to

accommodate several fluids and allow the user to select a fluid. This is further described in Section 4.2.

2. Treatment of dissolved noncondensable gas: The experimental data on performance of fluid discharge systems indicate that as the supply vessel depressurizes, dissolved gas comes out of solution and causes a slight delay in depressurization, thus delaying full discharge of the fluid. RELAP5 contains methods for transport of noncondensables, but does not explicitly account for presence of dissolved gas. This is further discussed in Section 4.3.

3. Modification of the constitutive relations: Many of the constitutive relations in RELAP5 are generically formulated, but use correlation coefficients derived from experimental data in water-steam systems. These need to be revised for alternate fluids, as needed.

4. Assessment against experimental data: ideally, using data for several different candidate fluids.

The above tasks are considered to be the major development efforts in adapting RELAP5 for alternate fluids and hence are the focus of the current development work. As the experimental program proceeds and additional data are collected, some additional tasks are considered likely, including:

5. Refinement of the choked flow model: This model controls the discharge flow rate for given upstream fluid conditions and hence is a significant contributor to the code performance.

6. Refinement of the constitutive relations based on assessment against data.

Based on discussions with NIST personnel, some additional code features have been identified as desirable. These are not currently being worked on, but expected to be once the above tasks have been completed. These are:

7. Allowance for liquid mixtures.

8. Allowance for powders transported by either liquid or gas carriers.

9. Refinement of flow-splitting model: In modeling parallel piping networks, RELAP5 does not explicitly recognize that direction changes, such as at Tee junctions, may alter the void fraction distribution. This may be important for piping networks that have significant length. There are some simple concepts that can be adapted to simulate non-symmetrical void fraction distribution. This task would explore these concepts.

Other tasks that have been defined are primarily from the perspective of user convenience, code maintenance and improvement of code execution time. These have been assigned lower priority at this time:

10. Elimination of unnecessary features that exist currently in RELAP5.

11. Modularization of subroutines.

12. Graphical user interface for input and output management.

The next sections, 4.2 and 4.3, describe the status of code development, with respect to Tasks 1 and 2 respectively. Prior to initiating Task 3, it was considered prudent to establish code configuration control and a workable quality assurance process. This is discussed in Section 4.4.

4.2   Implementation Of Fire-Suppressant Fluid Properties

As discussed previously, RELAP5 uses five (5) primary dependent state variables. These five state variables are

P: total pressure
α: gas phase volume fraction
U_g: gas phase specific internal energy
U_f: liquid phase specific internal energy
X_n: mass fraction of noncondensable gas in the gas phase

All thermodynamic variables are expressed in terms of the above five state variables. In addition, several state derivatives are needed for the numerical scheme. Section 4.2.1 presents the detailed requirements of the model fluid property package, for use with the proposed code.

4.2.1   Basic Thermodynamic Property Tables

Consider first the case without noncondensables. This is referred to as the Single-Component, Two-Phase Case.

A.   Single-Component, Two-Phase Case

Three sets of properties are required for this case.

Liquid Phase

The following are needed in the basic thermodynamic property package:

Temperature:	$T_f = T_f (P, U_f)$
Isobaric Specific Heat	$c_{pf} = c_{pf} (P, U_f)$
Isobaric Thermal Expansion Coefficient:	$\beta_f = \beta_f (P, U_f)$
Isothermal Compressibility:	$\kappa_f = \kappa_f (P, U_f)$
Specific Volume	$\upsilon_f = \upsilon_f (P, U_f)$
Specific Entropy	$s_f = s_f (P, U_f)$

The definitions for isobaric specific heat, isobaric thermal expansion coefficient and isothermal compressibility can be found from standard thermodynamic text books (e.g., Van Wylen and

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Sonntag, 1985). From these basic properties, the following derivatives are evaluated in the proposed code: density with respect to internal energy, temperature with respect to internal energy, density with respect to pressure, and temperature with respect to pressure.

Vapor Phase

Similarly, the following are needed in the basic thermodynamic property package:

Temperature:	$T_g = T_g(P, U_g)$
Isobaric Specific Heat	$c_{pg} = c_{pg}(P, U_g)$
Isobaric Thermal Expansion Coefficient:	$\beta_g = \beta_g(P, U_g)$
Isothermal Compressibility:	$\kappa_g = \kappa_g(P, U_g)$
Specific Volume	$\upsilon_g = \upsilon_g(P, U_g)$
Specific Entropy	$s_g = s_g(P, U_g)$

and the same derivatives for the liquid phase are evaluated for the vapor phase.

Saturation Properties

In addition to the phasic properties and derivatives, the saturation properties are needed for interface evaluation and extrapolation to metastable states (i.e., superheated liquid or subcooled vapor). Two tables are needed, one based on temperature and the other based on pressure, as follows:

a.   Give saturation temperature, T^s:

Saturation pressure	$P = P(T^s)$
Isobaric Specific Heat	$c^s_{pf} = c^s_{pf}(T^s)$
Isobaric Thermal Expansion Coefficient:	$\beta_f = \beta^s_f(T^s)$
Isothermal Compressibility:	$\kappa_f = \kappa^s_f(T^s)$
Specific Volume	$\upsilon_f = \upsilon^s_f(T^s)$
Specific Entropy	$s_f = s^s_f(T^s)$

where the superscript s denotes saturation state.

b.   Give saturation temperature, P:

Saturation Temperature	$T^s = T^s(P)$
Isobaric Specific Heat	$c^s_{pf} = c^s_{pf}(P)$
Isobaric Thermal Expansion Coefficient:	$\beta_f = \beta^s_f(P)$
Isothermal Compressibility:	$\kappa_f = \kappa^s_f(P)$
Specific Volume	$\upsilon_f = \upsilon^s_f(P)$
Specific Entropy	$s_f = s^s_f(P)$

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In addition, the derivative of the saturation temperature with respect to pressure is required. This is evaluated using the Clapeyron equation.

B.   Two-Component, Two-Phase Case

In the presence of noncondensable gases, the gaseous phase (mixture of vapor and noncondensable gases) is assumed to be a Gibbs-Dalton mixture of vapor (either treated as an ideal gas or from property tables) and ideal gases. Note that the noncondensable gases are present only in the gaseous phase.

An additional variable is calculated in RELAP5 for this case. It is the noncondensable quality, X_n, and is defined as the mass fraction of the noncondensable gases in the gaseous mixture, i.e.,

X_n = Mass of Noncondensable Gases / Mass of Gaseous Phase = M_n / ($M_n + M_s$)

where M_s is the mass of the vapor phase. The gaseous phase pressure is the sum of the partial pressure of each gaseous component, as usual. The equation of state for each noncondensable component is simply the perfect gas equation of state.

The liquid properties and derivatives are calculated in the same manner as described in Part A above. For the gaseous phase, the independent state properties are taken as P, U_g and X_n. All properties of the gaseous phase are expressed in terms of these three variables. Note that U_g is the specific internal energy of the gaseous phase, not just the vapor phase. The derivatives required are vapor temperature with respect to pressure, internal energy, and noncondensable quality, as well as interface temperature with respect to pressure, internal energy and noncondensable quality. The interface temperature, T_I, is based on the partial pressure of the vapor,

$T_I = T_I (P_s)$

The evaluation procedure for the above derivatives are relatively complicated. A detailed discussion is given in RELAP5-1, 1995. It suffices to mention that the proposed code contains the necessary coding for the evaluation procedure.

4.2.2   Generation Of Property Tables

As presented in Section 4.2.1 above, data are required for single phase properties as well as saturation properties in the solution scheme of the proposed code. These data can be in tabulated form. It would be preferable, if possible, to also supply any empirical correlations, curve fits, and canonical functions (in terms of Gibbs free energy and/or Helmholtz free energy), if known. If in tabulated format, the data will be reformatted to be consistent with the proposed code structure. If generating equations are available, these could be used to generate the data in the desired code format. Once generated, these property tables (in binary format) are used to

compute properties at any given pressure and internal energy through iteration, interpolation or both. The proposed code contains the necessary coding to perform this computation.

4.2.3 Thermal Transport Properties

Besides thermodynamic properties, a number of transport properties are needed for the candidate fluid. These include:

1.	Dynamic viscosity	$\mu_{f \text{ or } g} = \mu_{f \text{ or } g}(T,P)$
2.	Thermal Conductivity	$k_{f \text{ or } g} = k_{f \text{ or } g}(T,P)$
3.	Surface Tension	$\sigma = \sigma(T,P)$

These are computed in RELAP5 as functions.

4.2.4 Implementation Of The Property Tables Into Proposed Code

Various fluids have previously been implemented into the RELAP5. Examples are blood, ammonia, liquid sodium and lithium. As a result, RELAP5 has been set up to facilitate the implementation of a new fluid. Once the coding is understood, a new candidate fluid can be implemented into the proposed code. The procedure of incorporating a new fluid into RELAP5 is summarized as follows:

1. The user specifies the number of pressure and temperature points that will be used for the property tables, and the values of these points. These temperature and pressure points are to be entered following a prescribed format.

2. The required tables are generated via a program which contains the necessary formulae, empirical correlations, canonical functions, etc. The output from this program contains:

    a. saturation properties as a function of pressure
    b. saturation properties as a function of temperature
    c. single phase properties as a function of pressure and temperature

    For light water substance, for instance, this particular program calls other subroutines that calculates the Gibbs and Helmholtz functions as given in the 1967 ASME steam tables (Meyer et al, 1997). These subroutines are in object form in the transmittal package. For the candidate fluid, all information can be included in the generating program and hence avoiding the need for additional subroutines.

3. The output from the generating program is the required property tables for use in RELAP5. The format of the output file is as follows:

    a. Echo back the user input temperature and pressure points.

b. Tabulate the statistics of the table including number of temperature points, number of pressure points, number of saturation temperature points, number of saturation pressure points, and number of words in the binary file.

c. Saturation properties versus temperature as discussed before.

d. Saturation properties versus pressure as discussed before.

e. Thermodynamic properties versus pressure and temperature. For each pressure in the user supplied pressure range, the properties for each temperature

The above information is also written to a binary file. The proposed code uses this binary file for property computation. Once this binary file is available and linked to the code executable, the proposed code will be able to calculate the thermal hydraulic response of the candidate fluid undergoing a prescribed transient.

4.2.5 Halon 1301 Binary Data File Generation

As an example, this section presents a sample generation program for Halon 1301. The basic property relations are accessed from the REFPROP V. 4.0 software package (Gallagher et al, 1993). REFPROP is a calculation package for a wide variety of refrigerants, including Halon 1301 and the potential candidate fluid R227ea. Halon 1301 was chosen as a test case for implementation because there is experimental data readily available to check out the implementation method.

The major undertaking is to interface the appropriate subroutines in REFPROP with the coding in the generation program. RELAP5 expects three property tables: (i) saturation properties given temperature, (ii) saturation properties given pressure, and (iii) single phase properties versus temperature at a given pressure value (i.e., isobar). The values of pressure and temperature are supplied by the user and are input to the generation program. The needed properties include specific volume (m^3/kg), internal energy (J/kg), thermal expansion coefficient (1/K), isothermal compressibility coefficient (1/Pa), constant pressure specific heat (J/kg-K) and entropy (J/kg-K).

Figure 4.1 shows the flow chart of the generation program. The major steps of the program are described below:

1. The critical states (pressure, temperature and specific volume) as well as the minimum and maximum allowable values are supplied via data statements.

2. The user supplied temperature and pressure values are read. The input data are examined to ensure that they are within the minimum and maximum limits specified in Step 1 and are in ascending order.

3. Various pointers and table statistics are calculated.

4. Call Subroutine *table3* to generate the saturation table as a function of temperatures.

5. Call Subroutine *table4* to generate the saturation table as a function of pressures.

6. Call Subroutine *table5* to generate the single phase tables as a function of temperature for a given pressure.

7. Write output to an ASCII file and a binary file.

The interface with REFPROP are accomplished with the following steps:

1.   In the main program, initialize the REFPROP subroutines.

2.   In Subroutine *table3*:
   a.   Calculates the saturation pressure, specific volume, enthalpy, constant pressure
         specific heat, and specific entropy of each phase, by calling appropriate
         subroutines in the REFPROP package. The internal energy is then calculated
         from (h - pv), where h is the enthalpy, p is the pressure and v is the specific
         volume. Finally, the thermal expansion and isothermal compressibility
         coefficients are estimated by numerical differentiation. Thus, for the thermal
         expansion coefficient, the following is calculated

   $$\beta_f = (1/\upsilon_f) [\upsilon_f \upsilon_f (T\text{-}dT, p)]/dT \text{ along an isobar, and}$$

   $$\beta_g = (1/\upsilon_g) [\upsilon_g (T\text{+}dT, p) - \upsilon_g]/dT \text{ along an isobar.}$$

   For the isothermal compressibility coefficient, the following is calculated

   $$\kappa_f = -(1/\upsilon_f) [\upsilon_f (T, p\text{+}dp) - \upsilon_f]/dp \text{ along an isotherm, and}$$

   $$\kappa_g = -(1/\upsilon_g) [\upsilon_g - \upsilon_g (T, p\text{-}dp)]/dp \text{ along an isotherm}$$

   Currently, dT and dp are set at 1 K and 1 kPa respectively. The single phase
   specific volumes: $\upsilon_f (T\text{-}dT, p)$, $\upsilon_g (T\text{+}dT, p)$, $\upsilon_f (T, p\text{+}dp)$ and $\upsilon_g (T, p\text{-}dp)$ are
   also calculated by calling appropriate subroutines in the REFPROP package.

3.   In Subroutine *table4*:

   The process described in Subroutine *table3* above is repeated here, except that the
   saturation temperature is calculated given the pressure value.

4.   In Subroutine *table5*:

   In this subroutine, the fluid state is first determined by comparing the given temperature
   to the saturation temperature to determine the fluid state. The corresponding single phase
   properties (the specific volume, enthalpy and hence internal energy, constant pressure
   specific heat, and entropy) are then calculated by calling appropriate subroutines in the
   REFPROP package. Finally, the thermal expansion and isothermal compressibility
   coefficients are estimated using the procedure as discussed in Item 2 above.

The exact calling sequence of each of the REFPROP subroutines is described in the Users'
Manual of REFPROP.

In addition to generating the binary property data file, several modifications are needed to enable RELAP5 to execute on a fluid different than water. These modifications include:

1. Increasing the number of fluid types
2. Adding the name of the fluid (e.g., "halon") to the fluid type information
3. Modifying the thermal and transport property subroutines

With the above modifications, and the data file, RELAP5 can be used to simulate systems containing Halon 1301. To validate the modifications and to ensure the data file is interfaced properly with RELAP5, the following validation steps were taken:

1. Verify that the code modifications perform as designed and do not affect the code inadvertently. This is accomplished by running a test case with Halon 1301 as the fluid type and comparing the code calculated results with the property data file. To verify that the new coding did not affect other parts of the code, a test case with water as the fluid type is simulated. The results are compared to those of the same case simulated with the unmodified base code version. The two sets of results should be identical.

2. Verify the correctness of the interpolation subroutines for fluid types other than water. This is partially accomplished in Part 1 above. A comprehensive assessment of these interpolation subroutines is performed by developing a driver program to execute each of the interpolation subroutines interactively, and comparing the results to the results obtained by running the code.

3. Verify the correctness of the property data file. This is accomplished by comparing the results in the ASCII output data file with the results directly from REFPROP.

This validation was conducted using Halon 1301 as the test case. The results of the validation have confirmed that the modifications and data file have been correctly implemented, and that the various interpolation subroutines in the code perform as designed.

4.3   Sample Application

The adequacy of the modified code is confirmed by assessing the code against analytical problems and experimental data. A sample blowdown problem has been simulated. The problem consists of a bottle of 2760 cc in volume, containing liquid Halon 1301 at 5.71 MPa and 21 °C. The Halon is pressurized with nitrogen. Approximately 60% of the bottle is Halon 1301. The bottom of the bottle is fitted with a 77 mm^2 discharge nozzle. The Halon/nitrogen mixture is discharged into atmosphere. This problem corresponds to Test 146 contained in Elliott et al, 1984.

In code simulation, the bottle is represented by a Pipe component with 10 equal length cells, discharging to a constant pressure (1 atm) boundary condition. Figures 4.2 to 4.4 shows the simulation results. Figure 4.2 shows the calculated bottle pressure response compared to data. The bottle pressure was the only measured parameter reported for this test. Note that the characteristic pressure recovery due to nitrogen release from the Halon solution seen in the data is not captured in this simulation. This is because the Halon is assumed as a pure liquid in this calculation. This may also contribute partly to the underprediction of the depressurization rate.

Figure 4.3 shows the junction void fraction at the discharge nozzle. As seen, the nozzle is uncovered at about 1.0 second (i.e., the discharge flow becomes single phase gas/vapor). Also, for about 0.1 second, the discharge flow is mainly liquid.

Figure 4.4 shows the discharge flow rate. The maximum flow rate reaches about 6.0 kg/s. The discharge coefficients in this calculation have been set at unity for subcooled, two-phase and single-phase vapor critical flow. Assessment results (against water data) in the literature have shown that use of non-unity discharge coefficients is more appropriate. In addition, the orifice in the test may need a discharge coefficient less than 1.0. This modeling uncertainty and other code uncertainties will be considered in the assessment of the product code against data, and guidelines developed for design applications of the code.

The calculation presented in this section represents a preliminary scoping calculation. It demonstrates that the modified code version is able to produce reasonable results. A more comprehensive assessment will be conducted against both Halon 1301 and candidate fluid test data as the major development tasks are completed and experimental data is obtained.

4.3.1   Nitrogen Release Model

As mentioned above, RELAP5 does not account for dissolved noncondensable gases in the liquid phase. During blowdown of the fire-suppressant fluid, dissolved nitrogen will come out of solution and repressurizes the vessel. This has been observed in halon blowdown tests. The repressurization affects the subsequent pressure response, and the blowdown time. It is therefore necessary to account for the effects of nitrogen release from solution, in order to accurately model the blowdown process.

Fundamentally, the conservation equation for the noncondensable phase needs to be modified to account for the release of the dissolved component, via the source term (i.e, the right hand side of Equation 4.1-7). The resulting numerical solution procedure will be affected, and this requires significant code modification.

At the present time, instead of modifying the conservation equations, an alternate method is proposed. In this method, the dissolved nitrogen (noncondensable) is explicitly injected into the liquid volume via user input when the vessel pressure is sufficiently low. The amount of the injected nitrogen is determined from the initial amount of nitrogen dissolved in the solution at the initial conditions. The code input allows the user to provide a defined initial amount of noncondensable gas in each control volume. The following discusses this method.

Steps of Proposed Method

The following discussion assumes nitrogen as the noncondensable gas, and halon as the fire-suppressant fluid.

1. Calculate the amount of dissolved nitrogen at the initial conditions.

    a. Given P_i, T_i, initial liquid volume V_i

    b. Get partial pressure of halon, neglecting the influence of the dissolved nitrogen in the liquid phase. Hence,

    $$P_{b0} = P_{halon} = P_{sat @ Ti}$$

    where P_{b0} is the partial pressure of halon in the gaseous space if there were no dissolved nitrogen, and $P_{sat @ Ti}$ is the saturation pressure of halon at the initial temperature T_i.

    c. Get partial pressure of nitrogen. From Raoult's law, the partial pressure of halon vapor in the presence of dissolved nitrogen in the solution is given by

    $$P_b = P_{b0} (1 - H P_a)$$

    where P_{b0} is calculated from b) above, H is the Henry's law constant, and P_a is the partial pressure of nitrogen. The total pressure P_i is composed of the partial pressures. Hence

    $$P_b + P_a = P_i$$

    Solving the two equations for P_a, one obtains

    $$P_a = (P_i - P_{b0}) / (1 - H P_{b0})$$

    The Henry's law constant is empirically given by

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$$H^1 = a + bT + cT^2 + dT^3$$

    d.   Calculate mass of halon at the initial conditions.

$$M_b = \rho_b V_i$$

where ρ_b is the density of liquid halon.

    f.   Hence mass of nitrogen initially dissolved is

$$M_a = \alpha M_b$$

2.   Calculate the nitrogen release pressure. At the point of nitrogen release, the pressure difference across a micro bubble of diameter D is given by

$$\Delta P = 4\sigma/D$$

where σ is the surface tension. Initially, the nitrogen bubble is at P_i. As the vessel pressure drops during the blowdown process, the pressure outside the bubble decreases below P_i. However, the bubble remains stable under surface tension. When the pressure difference across the bubble reaches the value given above, the surface tension no longer is sufficient to maintain a stable bubble. The bubble grows, and its diameter increases. This in turns further decreases the pressure difference across the bubble and the bubble growth accelerates. The release pressure is then given by

$$P_{rel} = P_i - 4\sigma/D$$

3.   Inject the nitrogen at (P_i, T_i) over a prescribed time span (determined by the performance and data comparison), into the liquid filled region. This is to simulate the nitrogen release behavior as discussed above.

This approximate procedure has been applied to Test 146. Figure 4.5 shows the pressure response for Test 146 taking into account dissolved nitrogen. The results show that, with this procedure, the code calculations exhibit the characteristic repressurization observed in the test, and demonstrate that the procedure functions as desired. Further assessment is planned to refine the procedure, and to more mechanistically treat dissolved gases coming out of solution. It is recognized that if this type of approximate procedure is eventually adopted , it needs to be implemented as part of the code. The user would probably be required to supply initial concentration levels in the input file.

4.4 Code Configuration Control And Pc Installation

It is expected that the proposed code will undergo additional modifications and model improvements to achieve the desired performance. To properly track the modification, and minimize error of application, it is necessary to implement some sort of code configuration control and quality assurance. In addition, the proposed operating platform for application is PC, for its wide usage and convenience. Currently, the Windows 95 operating system is selected. The following presents the code configuration control installation and PC installation of the proposed code.

4.4.1 Code Configuration Control

To facilitate code configuration control, a labeling system has been developed to track each change implemented into the base code to adapt the code for fire-suppressant fluids, as well as each interim version of the product code. Each change will be formally documented describing the change, the rationale for the change and the change number.

In addition, a plan has been adopted to assure adequate quality in the product code. This plan follows the guidelines of the DE&S software quality assurance procedures. The major ingredients of the plan are:

1. Documentation, including the theoretical manuals, the user's manual and the verification and validation (V&V) documentation. The theoretical and user's manual are the same as those for the base code RELAP5 (RELAP5-1, 1995 and RELAP5-2, 1995 respectively). Modification to the theoretical model, code structure, input requirements, and numerical scheme will be documented separately. For the Verification and Validation (V&V) documentation, a matrix of test cases will be executed to verify and validate each version of the proposed code as well as the base RELAP5 code. The calculated results will be compared to data, if applicable, and documented. The test cases are selected to assess the features of the code that are most important to the intended application, including the critical flow model, the interphase drag models, the state relationships, and noncondensable presence.

2. Second party verification of all documentation produced in Item 1 above.

3. Documentation and resolution of software errors. The USNRC information network will be periodically reviewed to identify potential errors associated with the base RELAP5 computer code. Each potential error will be assessed for its impact on the proposed code, if any. Any error which is judged to have an impact on the proposed software will be corrected, or otherwise noted in the documentation. Errors associated with the proposed code (i.e., errors associated with the changes made to the RELAP5 code to create the proposed code) will be assessed and resolved.

4.4.2 Installation Of Relap5/Mod3.2 On Windows 95

Idaho National Engineering and Environmental Laboratories (INEEL) transmitted the PC version of the RELAP5/MOD3.2 code to Duke Engineering & Services. However, the executable operates on the LINUX operating system (UNIX equivalent in PC). Since our goal is to use the Windows 95 operating system, the transmitted executable is not applicable. Instead, the installation began with the source code (PC version) transmitted separately from INEEL.

The hardware chosen for installation is a laptop having a Pentium PC 233 MHz Processor with 64 MB RAM and 3.2 GB Hard Disk drive. The compiler is the Digital™ Visual FORTRAN Compiler (Standard Edition) for Windows95.

Verification

The purpose of verification was to ensure that the code is installed properly on the designated operating system. A set of four problems representative of discharge from pressurized systems has been simulated. The results were compared to those obtained from the HP Workstation running on the HPUX 9.01 Operating System. Since the code has been extensively validated on various UNIX workstation platforms, this comparison is judged adequate in verifying the installation of the code on the PC Windows 95 platform.

The comparison showed that the PC/Win95 results match very closely the HP730 results. In most cases, no discernable differences between the two sets of the results can be detected.

Validation

The purpose of the validation is to ensure that the base code is able to reasonably simulate the expected behavior in the intended application. The primary areas chosen for validation are the interphase drag model and the critical flow model in the proposed code. One should be aware that the interphase drag model also affects the critical flow calculation, because it affects the void distribution which in turns affects the two-phase critical flow rate. Three tests based on experiments in water-steam systems were used for validation. The calculation results from these three tests generally demonstrate RELAP5's ability to model discharge from a pressurized vessel. However, the comparison also indicates areas that may potentially need improvement. This is not uncommon, based on previous experience with publicly released versions of RELAP5 and other similar codes. Part of the code development task is to conduct systematic code assessment against a spectrum of experiments and address code deficiencies found.

As an example, the assessment results for one test from the Marviken blowdown experiments (EPRI, 1982) are presented here. The test was a sudden depressurization of a large vessel filled initially with water at about 6 MPa. The vessel was vertical and the discharge occurred from the bottom through a nozzle equipped with a rupture disc. Figures 4.6 and 4.7 show the assessment results. Figure 4.6 shows the vessel pressure comparison. The initial dip in the vessel pressure is not captured by the code, but the subsequent depressurization rate is well predicted. The initial dip in pressure seen in the data is considered to be due to delayed nucleation at the blowdown nozzle. Figure 4.7 shows the comparison of the break flow rate. In general, RELAP5

underpredicted the flow rate. Since the depressurization is reasonably predicted (see Figure 4.6), the cause for this underprediction is believed to be due to overprediction of the break void fraction. Based on previous code assessment experience, this suggests that the interphase drag models in the code may need to be improved. This will be substantiated by further assesements and is part of Tasks 3 and 4 identified in Section 4.1.2. Even though this test was for a water-steam system, many of the code models that affect the calculation are generic. Hence comparison to data from water-steam systems can provide useful information for code development.

4.4.3   Summary Of Code Development Work On Pc

The base RELAP5 code has been installed on a PC Win95 platform. The compiler used is Digital Visual Fortran (Standard Edition). The installation started with the source code listing obtained from INEEL. Four test problems were used to verify and validate the installation of the code on the particular platform. The verification process involved comparing the PC results to the HP730 results. Since the code has been extensively executed on the HP Unix platform, it is justifiable to consider these results as valid bases for verification on other platforms. For all test problems considered, the PC results are practically the same as the HP730 results. Hence, the installation process has been verified.

Comparison of the PC results to test data, where applicable, was also made. Three of the test problems used were simulations of experiments. Thus code calculations could be compared to data. The comparison indicates the general applicability of the code for modeling discharge from a pressurized vessel. It also reveals certain short-comings of the code, particularly in the interphase drag models in the bubbly flow regime. Further assessment against data will be continuously performed during the development stage. Code modifications and user guidelines will be developed to address identified deficiencies.

5. PLANS FOR THE NEXT YEAR

The project started April 1st, 1998. The present report covers the period through the end of September 1998. It is expected that the project will continue for the duration of fiscal year 1999.

During the next 12-15 month period, we expect to accomplish all of the proposed project tasks. Specifically, we expect to accomplish the following:

- Verify further that dynamic measurements for mass flow rate, void fraction, and temperature are successful.
- Collect experimental data with CO_2 and FC-227ea at different driver pressures.
- Collect experimental data using other fluids if suggested by NIST program manager.
- Install CO_2 and FC-227ea properties into the code.
- Modify the code to accept treatment of dissolved non-condensable gas.
- Modify the constitutive relations in the code for the fire suppressants.
- Assess the code against experimental data.

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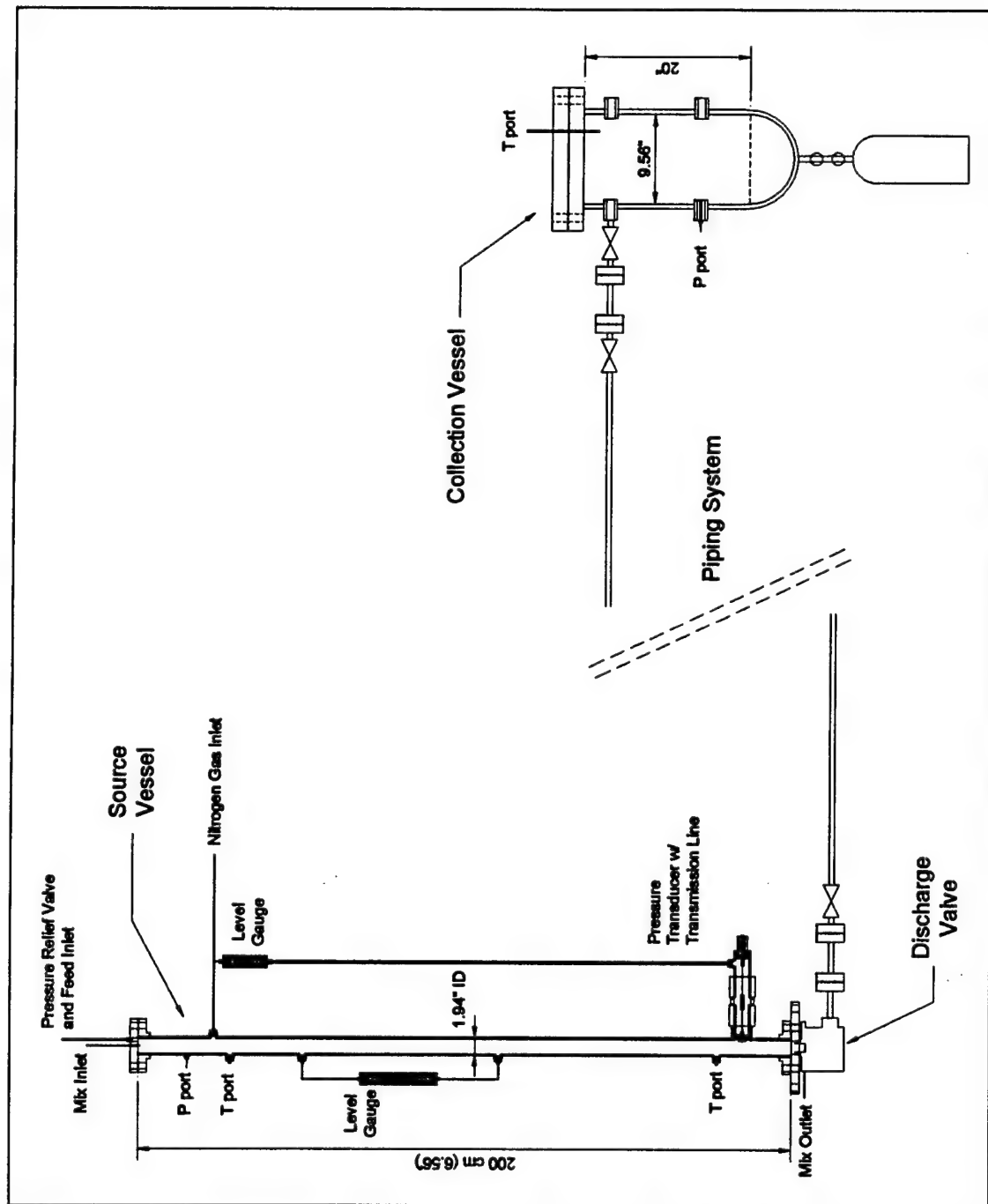
Figure 3.1: Side View of the Test Loop: Source Vessel, Discharge Piping, and Collection Vessel.
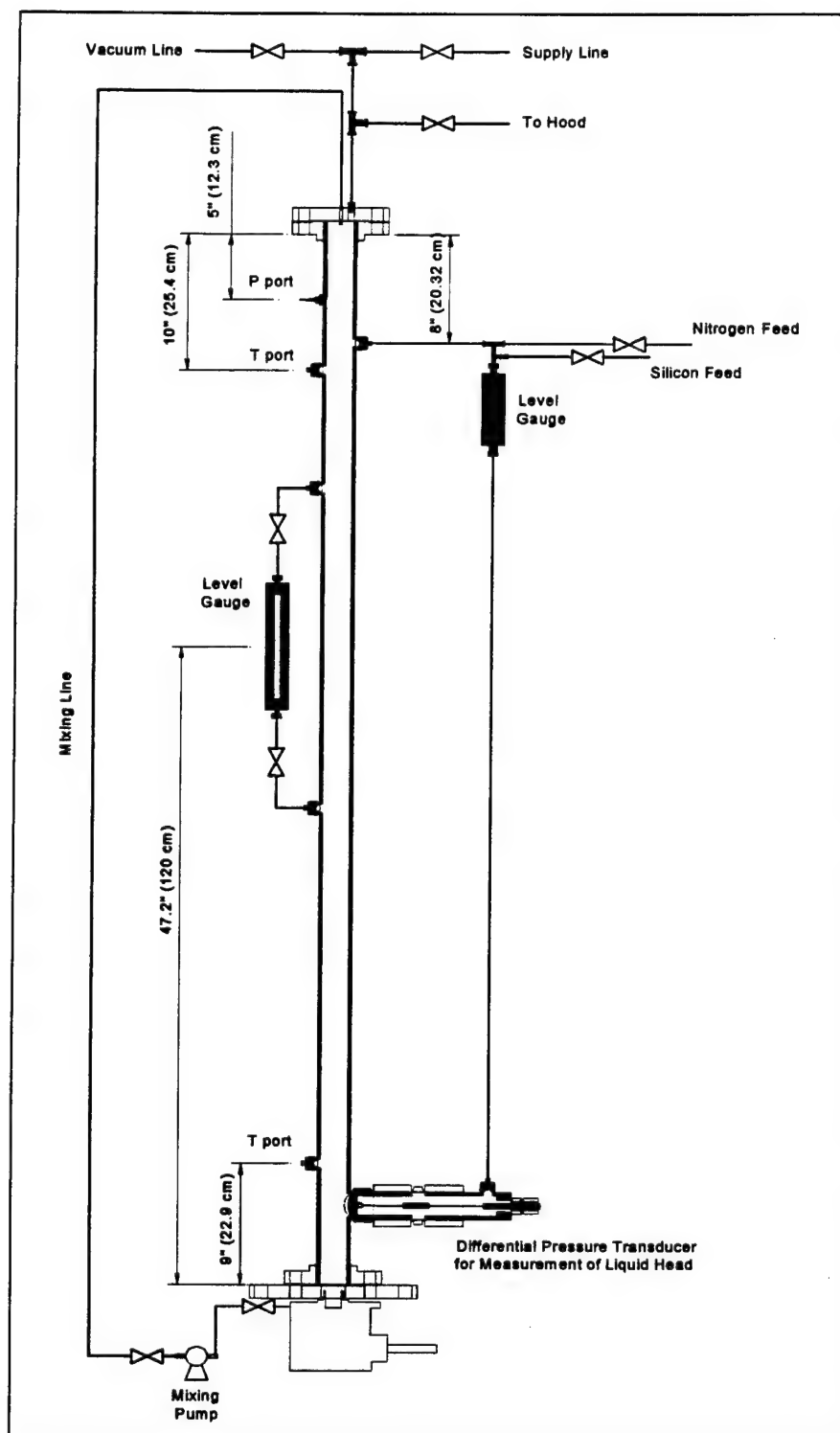
Figure 3.2: Schematic of Source Vessel.
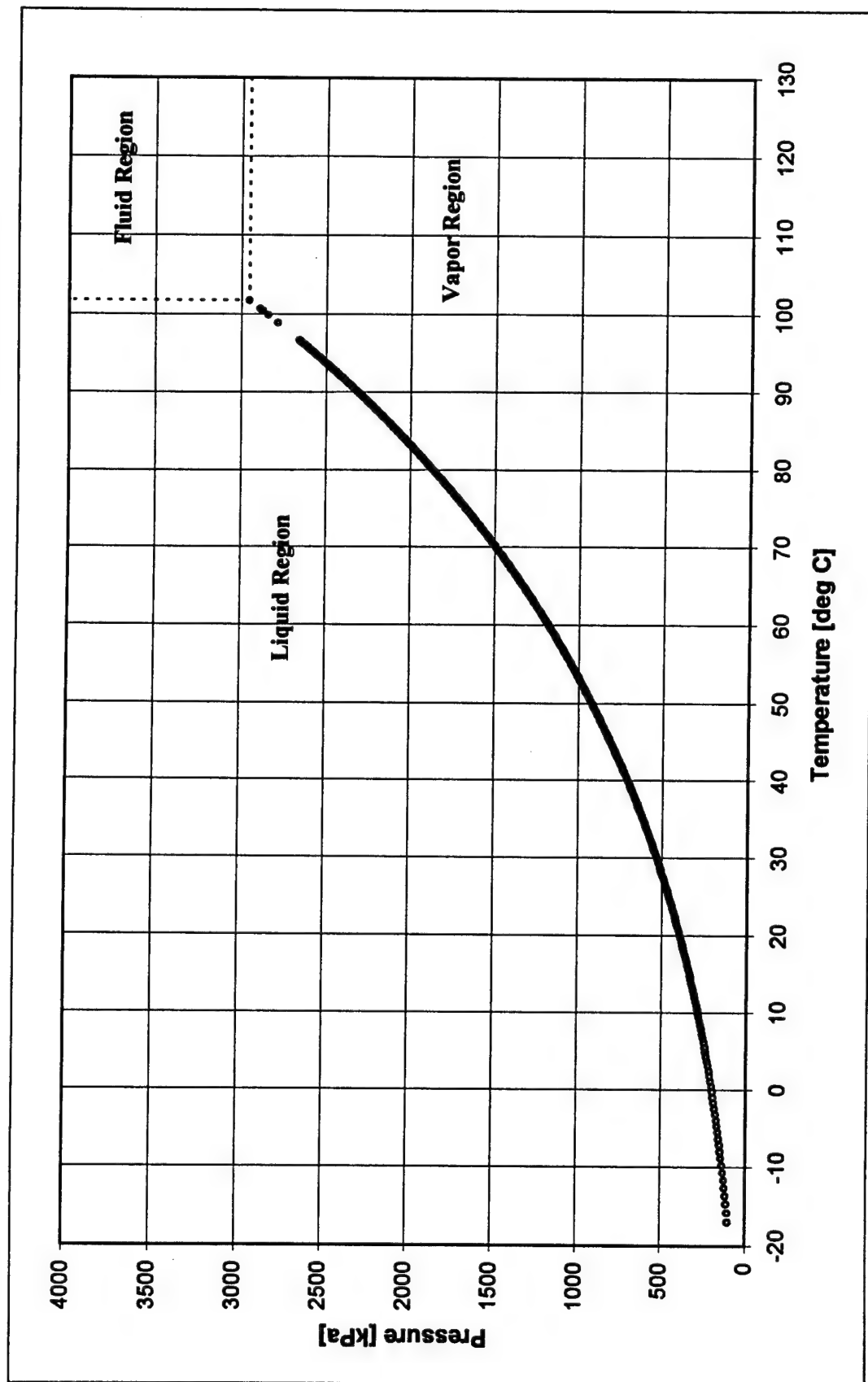
Figure 3.3: Pressure vs. Temperature Saturation Curve for FC-227ea.
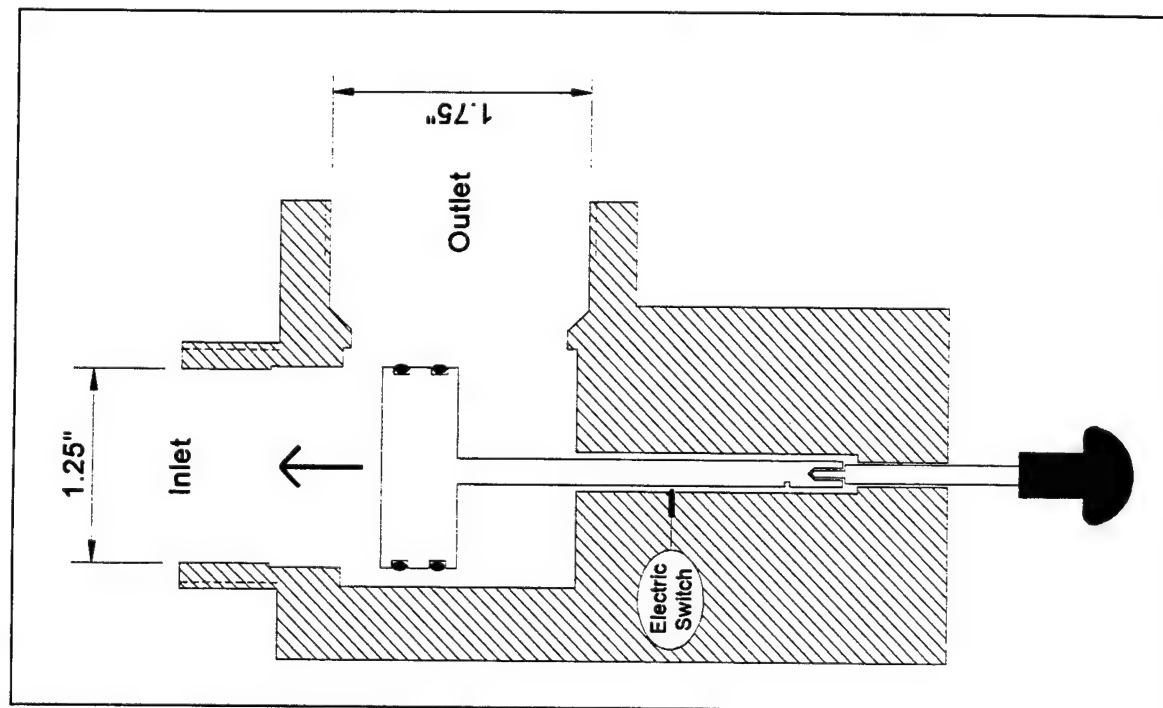
Figure 3.4: Schematic of Quick-Action Discharge Valve.
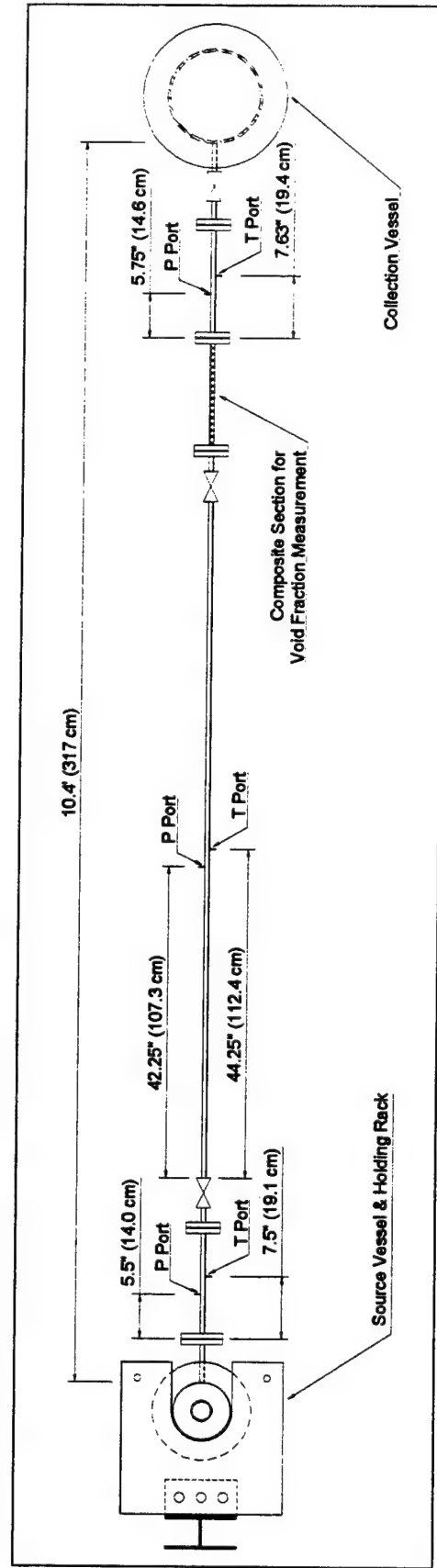
Figure 3.5: Top View of Test Loop, Schematic of Discharge Piping System.
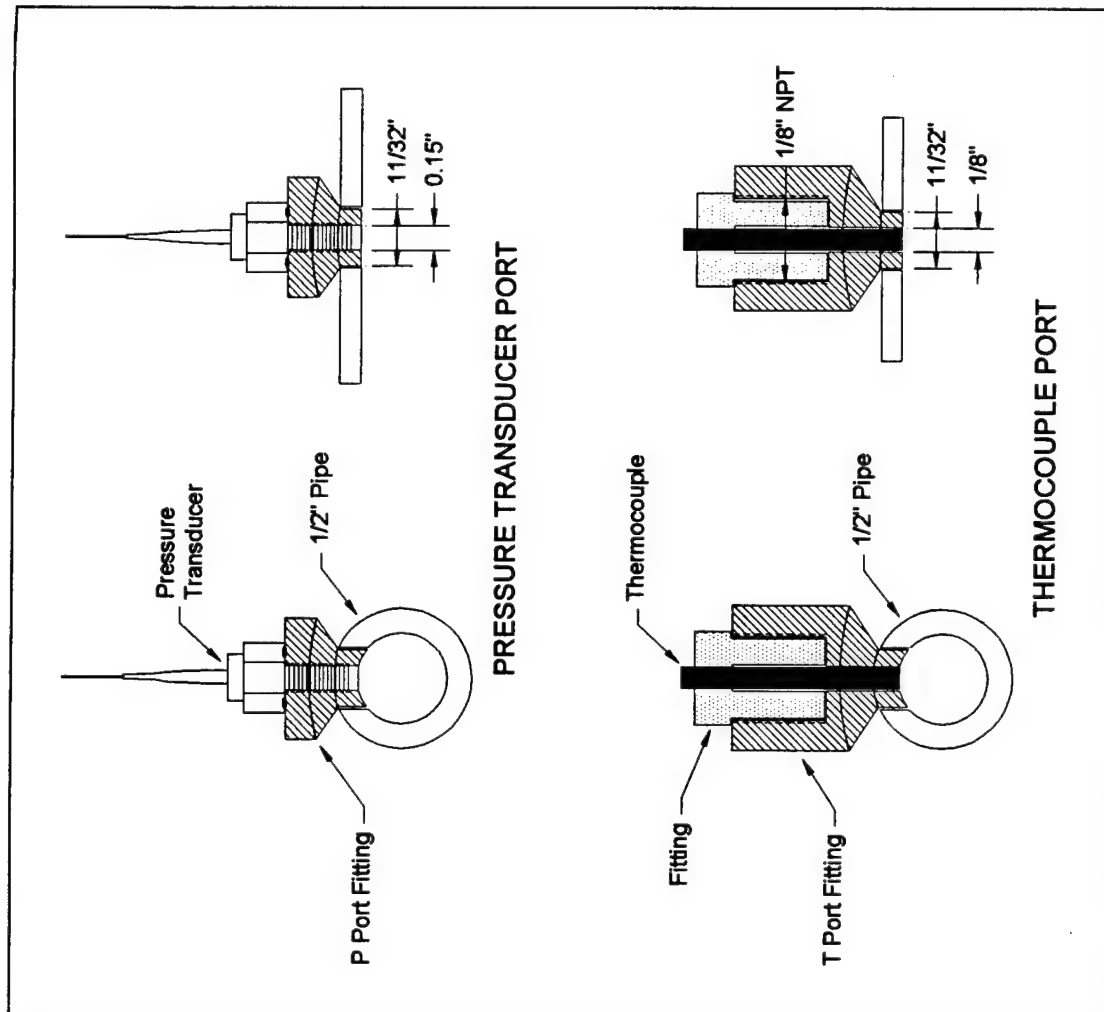
Figure 3.6: Schematic of Pressure Fittings for Temperature and Pressure Ports.
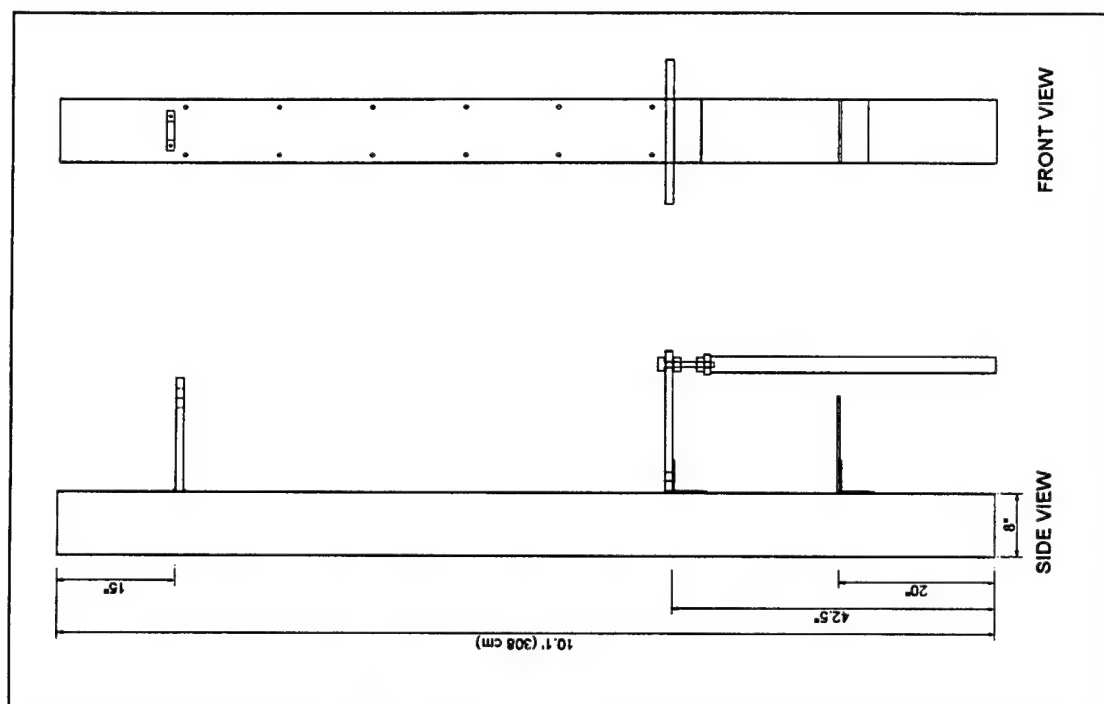
Figure 3.7: Schematic of Rack Used to Hold the Source Vessel.
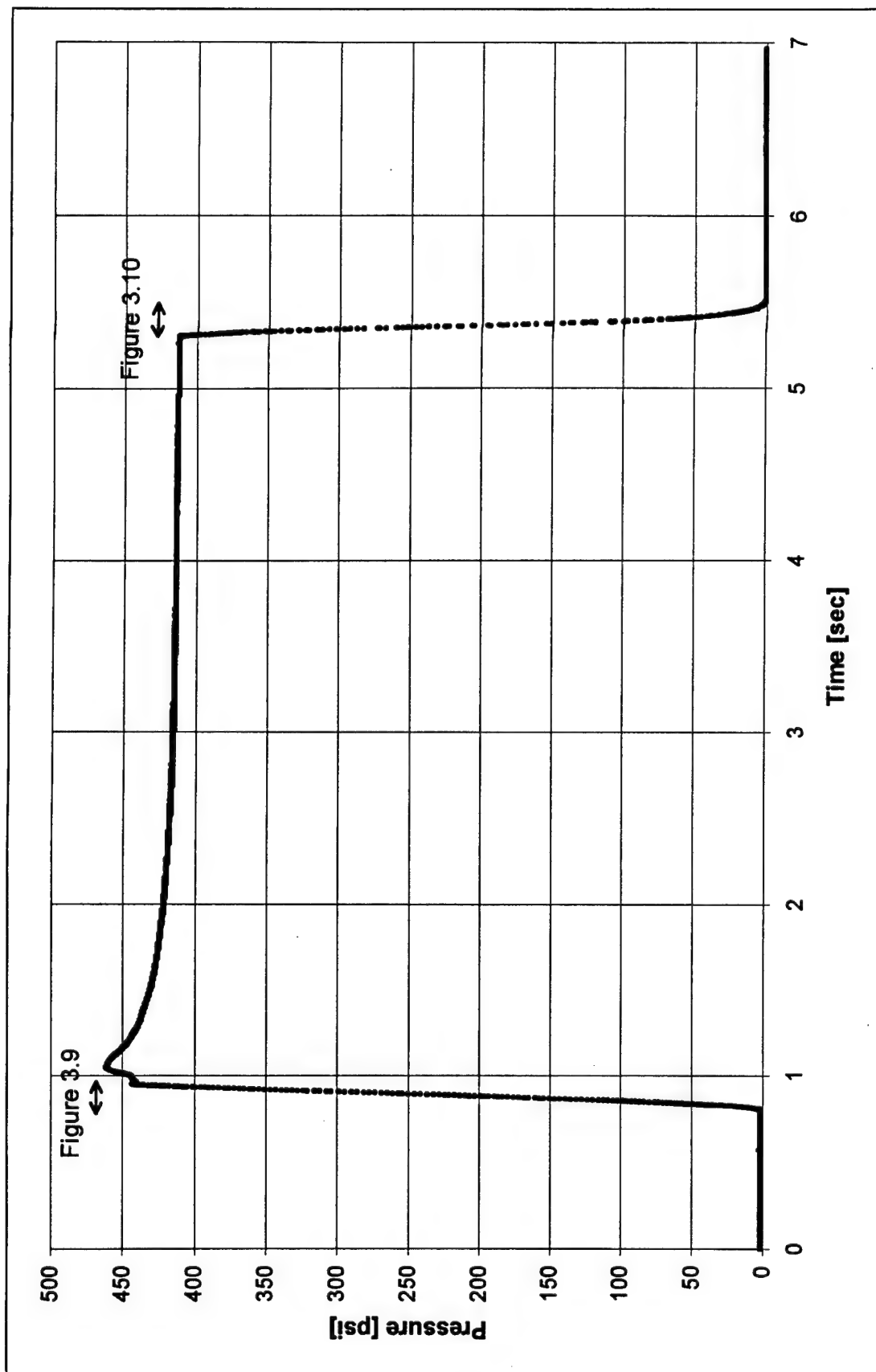
Figure 3.8: Pressure Histogram for Response Test with the 1000 PSIG Pressure Transducer.
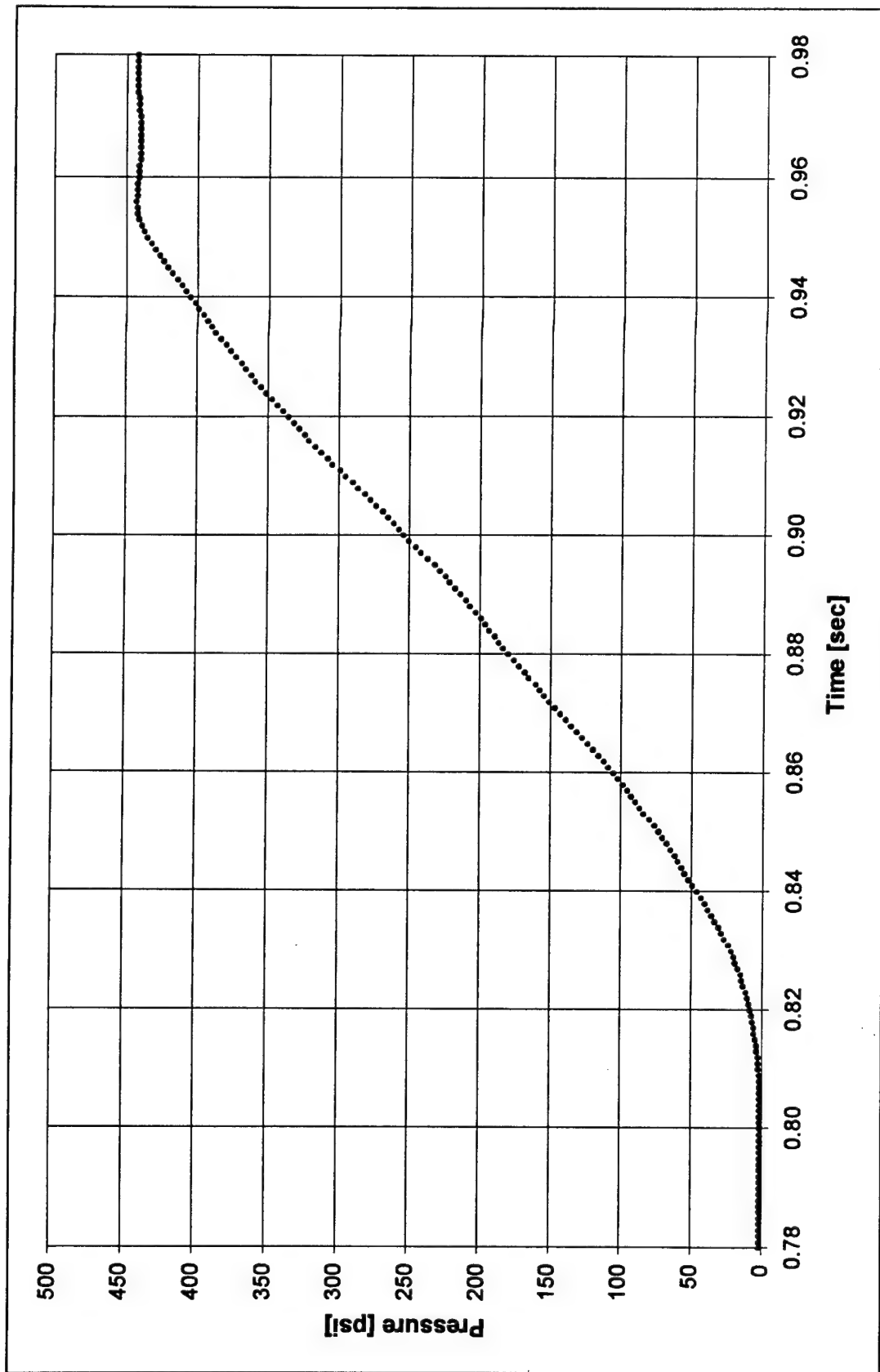
Figure 3.9: Response of the Pressure Transducer to Sudden Pressurization.
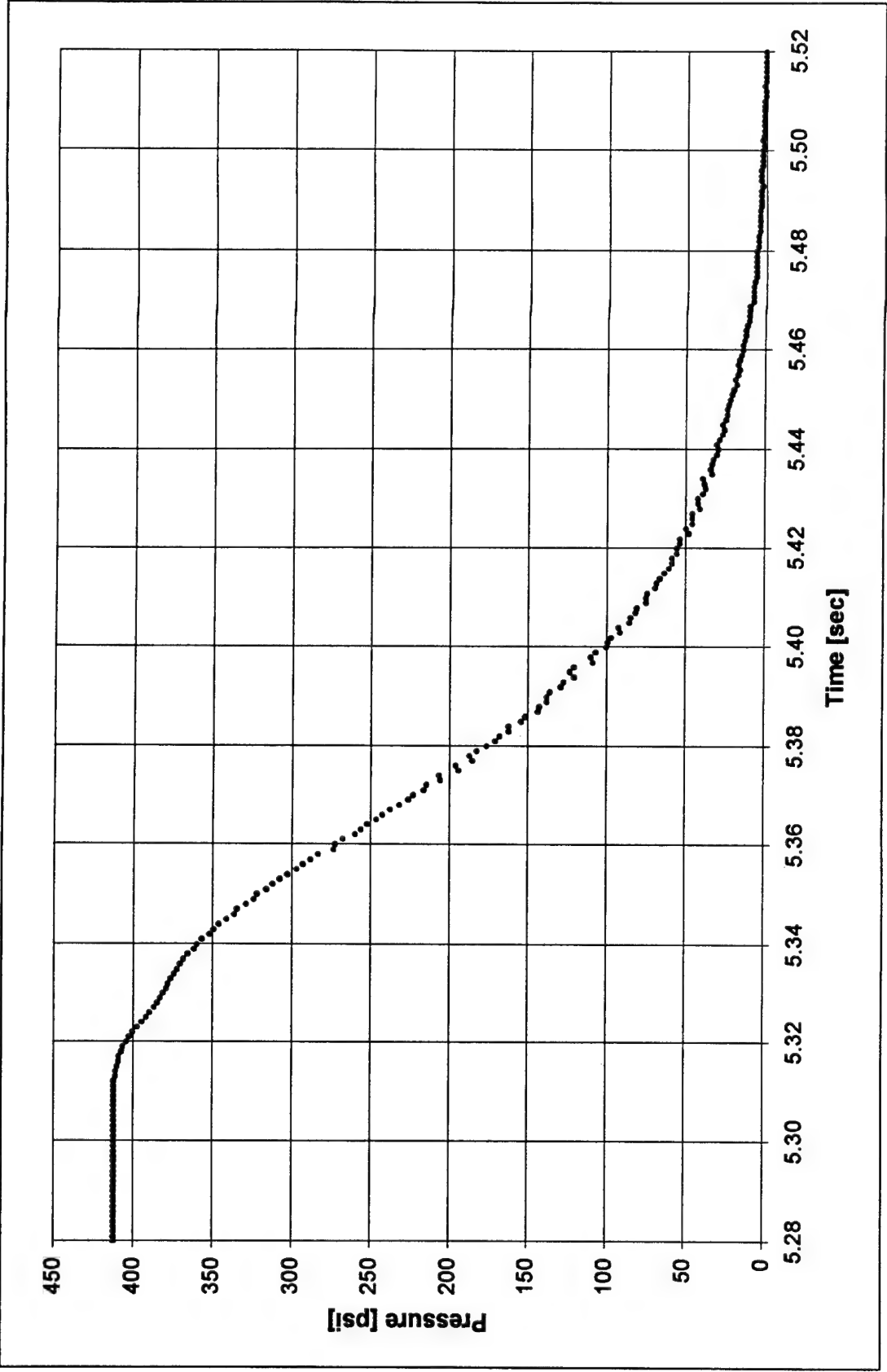
Figure 3.10: Response of the Pressure Transducer to Sudden Depressurization.
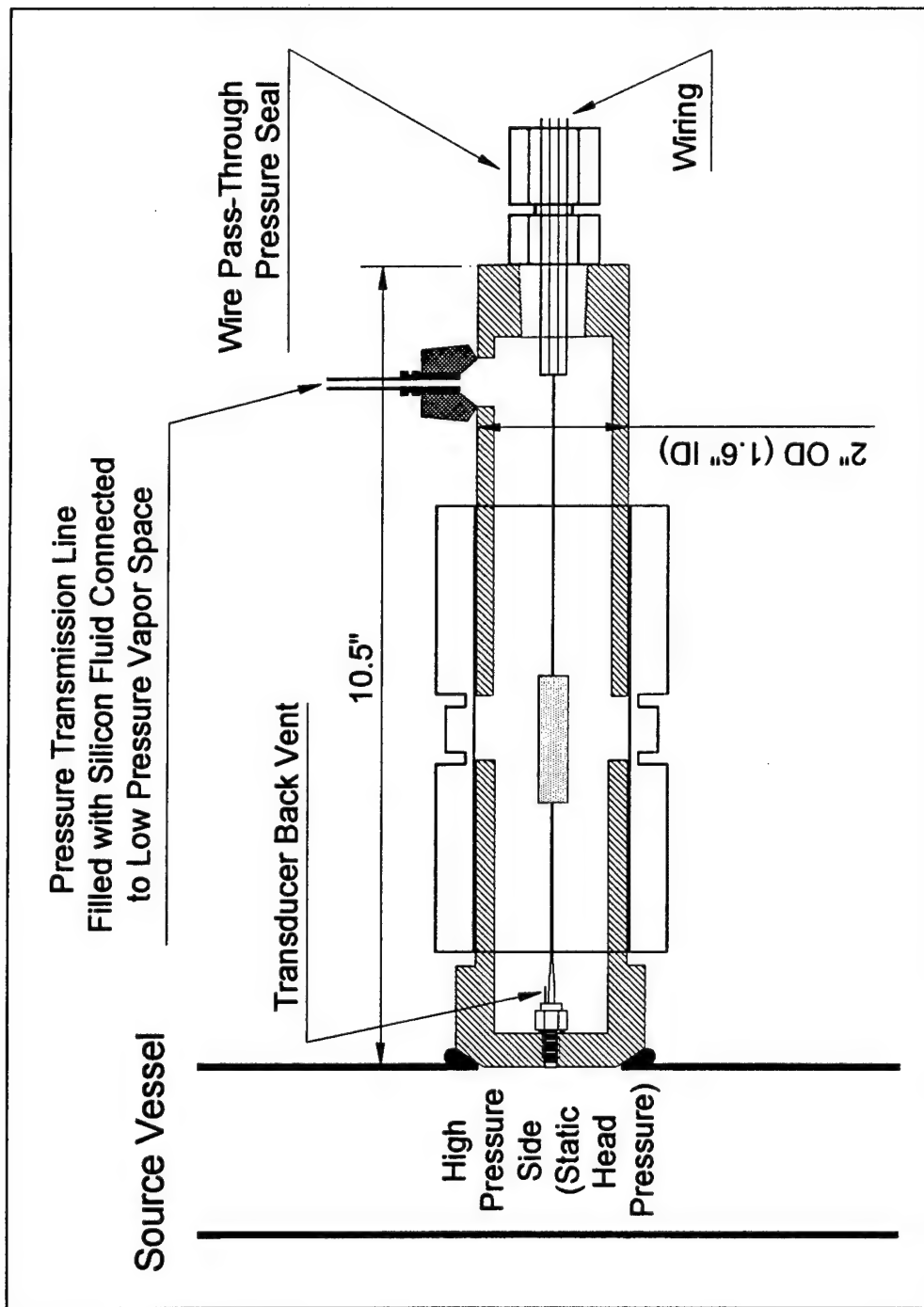
Figure 3.11: Schematic of the Differential Pressure Transducer and Transmission Area Used in Flow Rate Measurement.
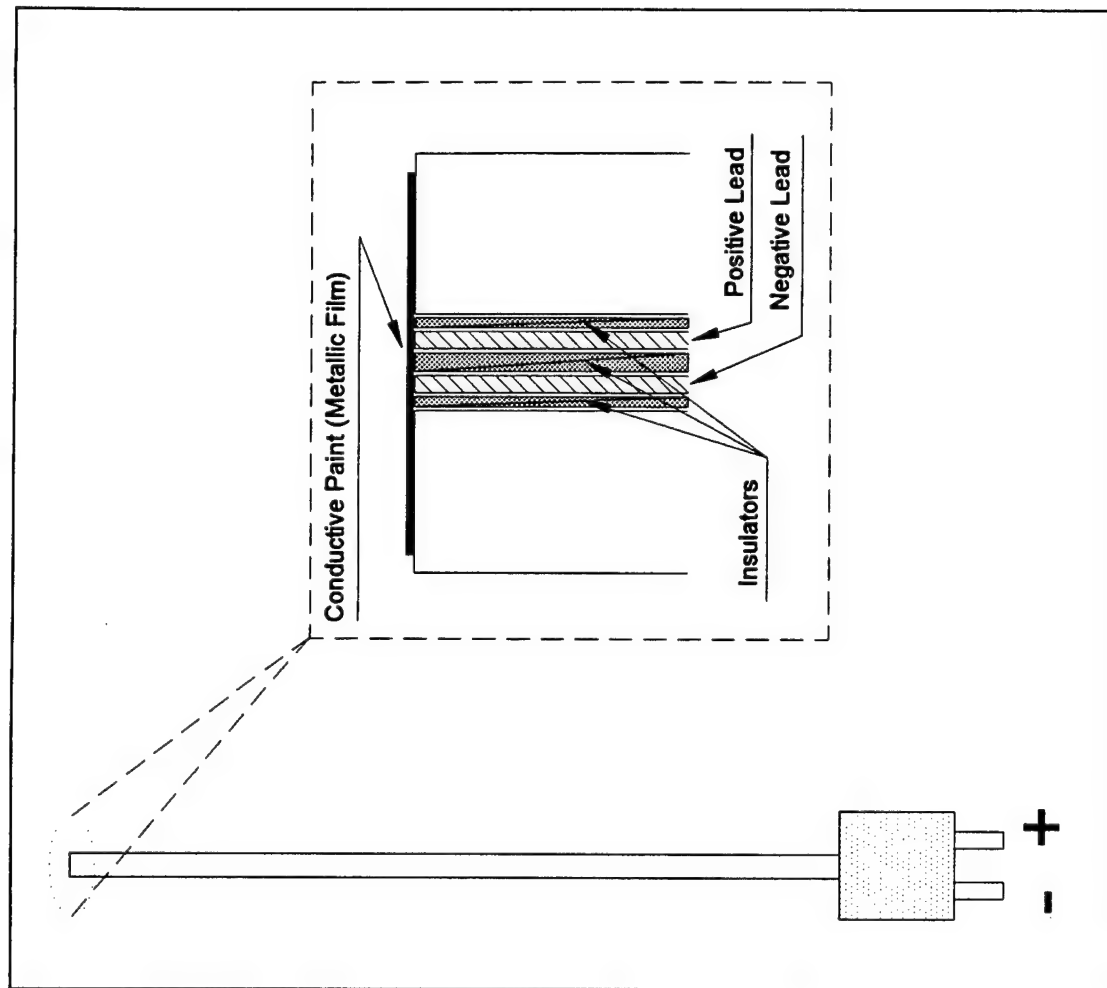
Figure 3.12: Schematic of the Film Thermocouple.
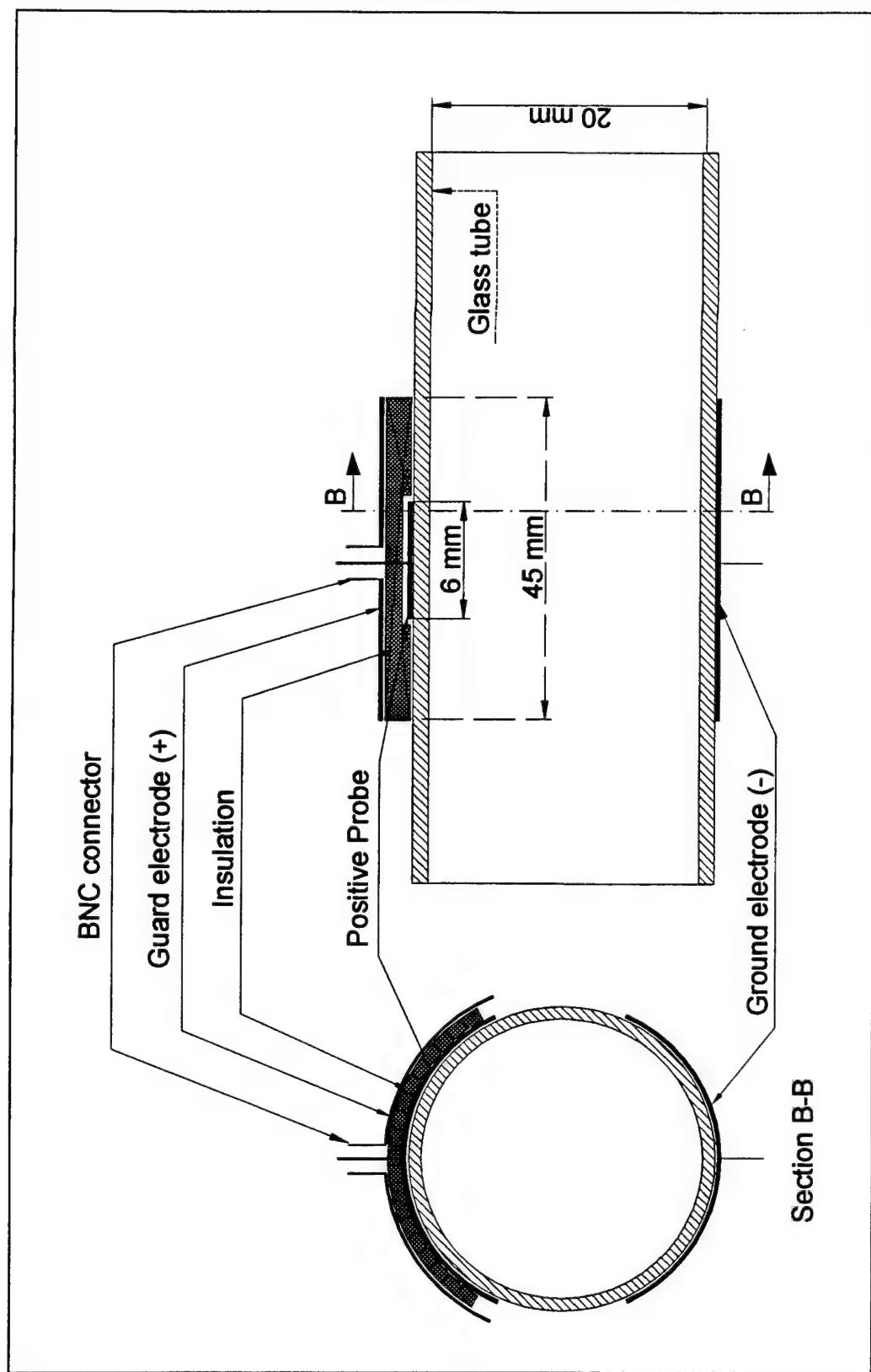
Figure 3.13: Schematic of the Capacitance Probe for the Measurement of Void Fraction.
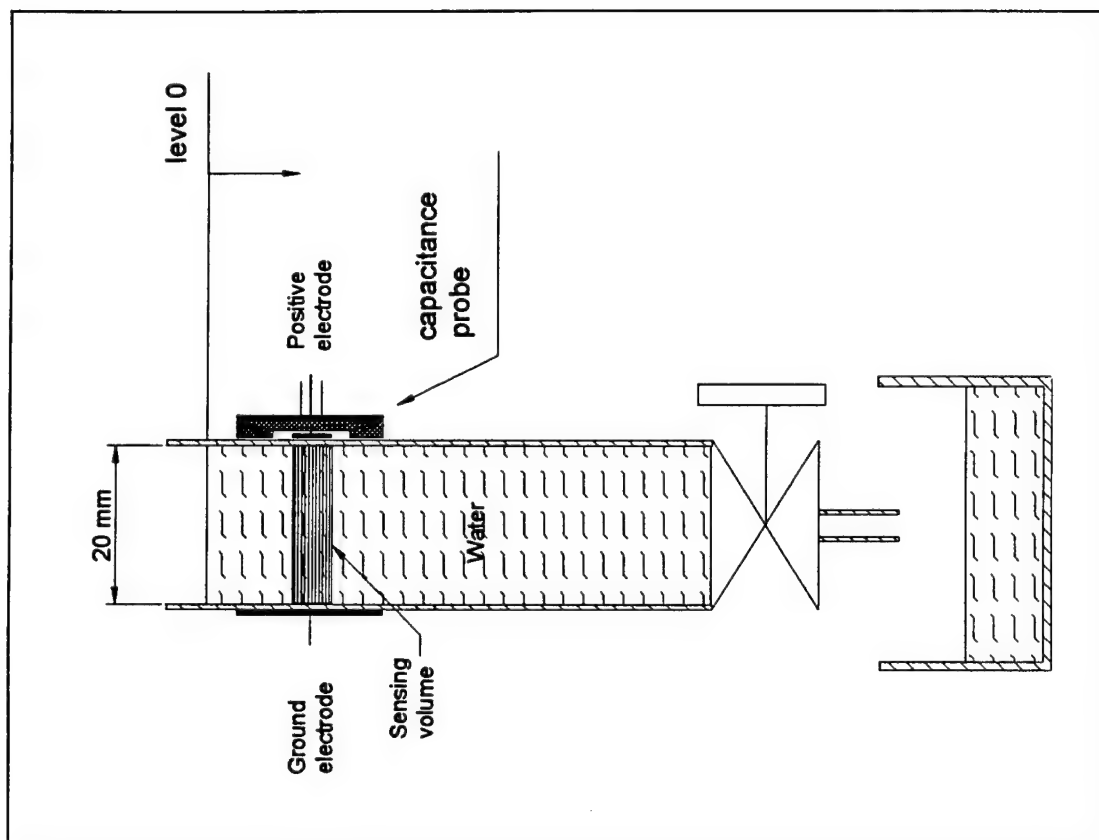
Figure 3.14: Bench Setup to Test the Capacitance Sensor.
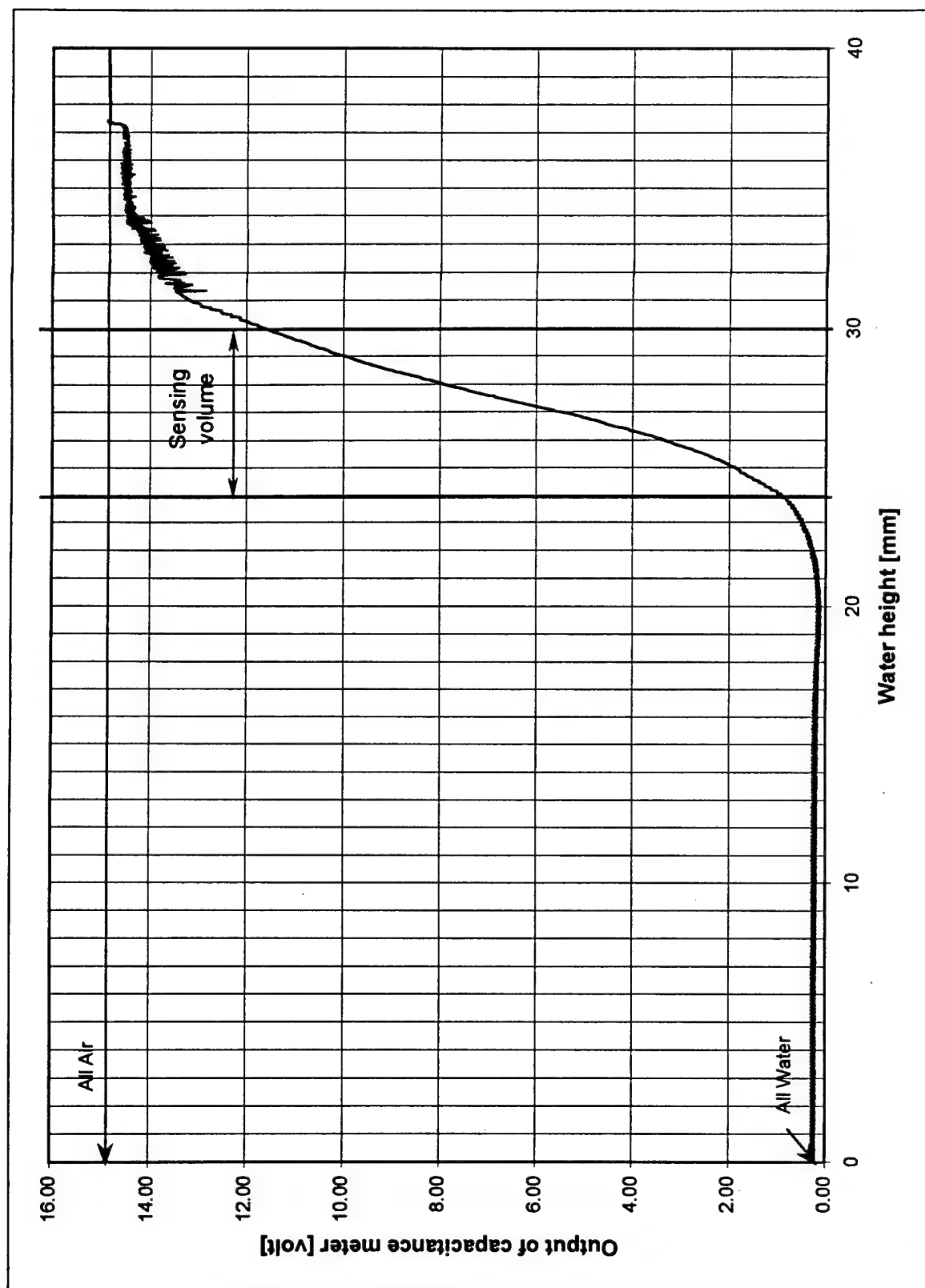
Figure 3.15a: Raw Data Capacitance Signals.
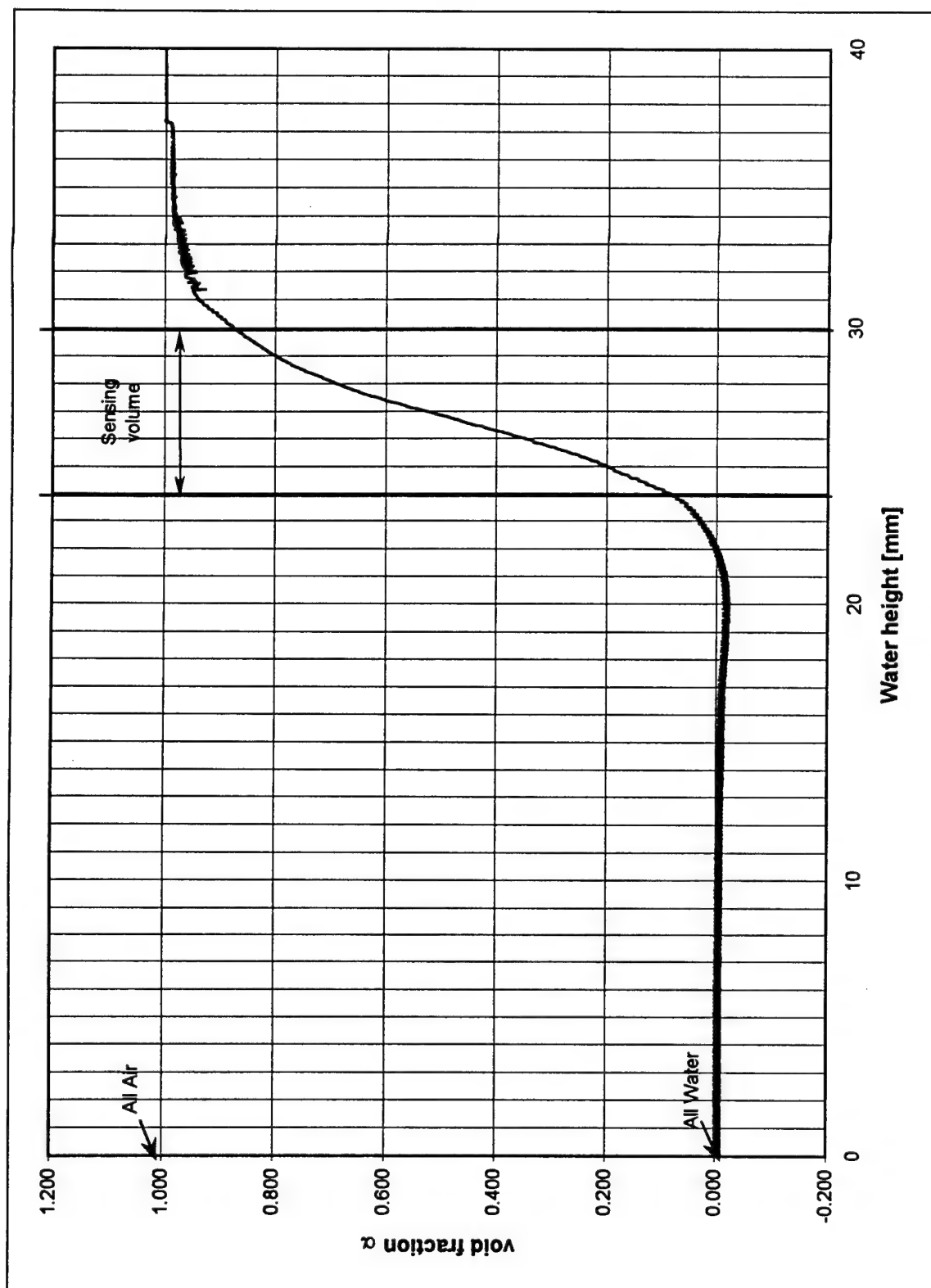
Figure 15b: Calculated Void Fraction from Capacitance Signals.

Figure 4.1: <u>Flow Chart of Generation Program</u>
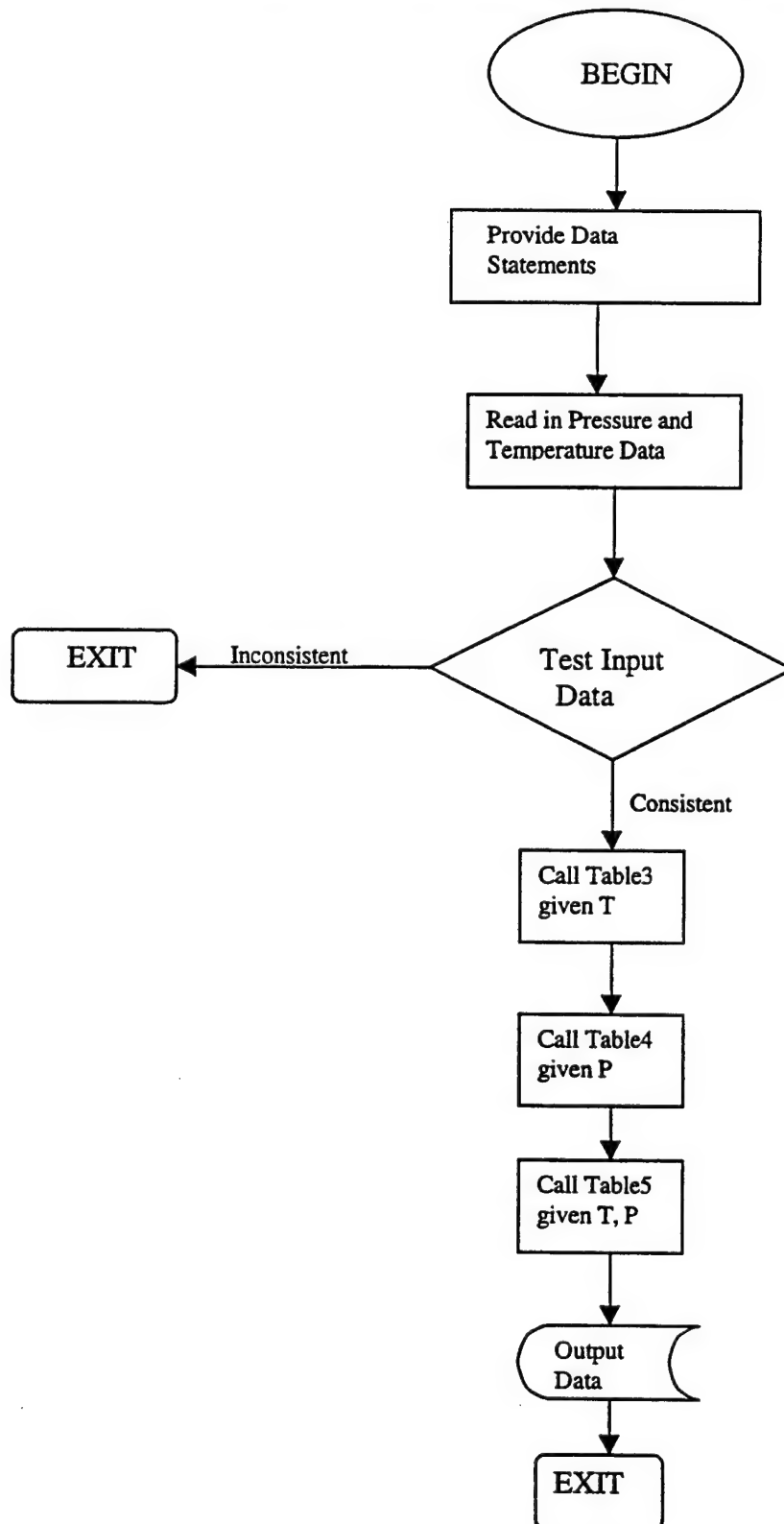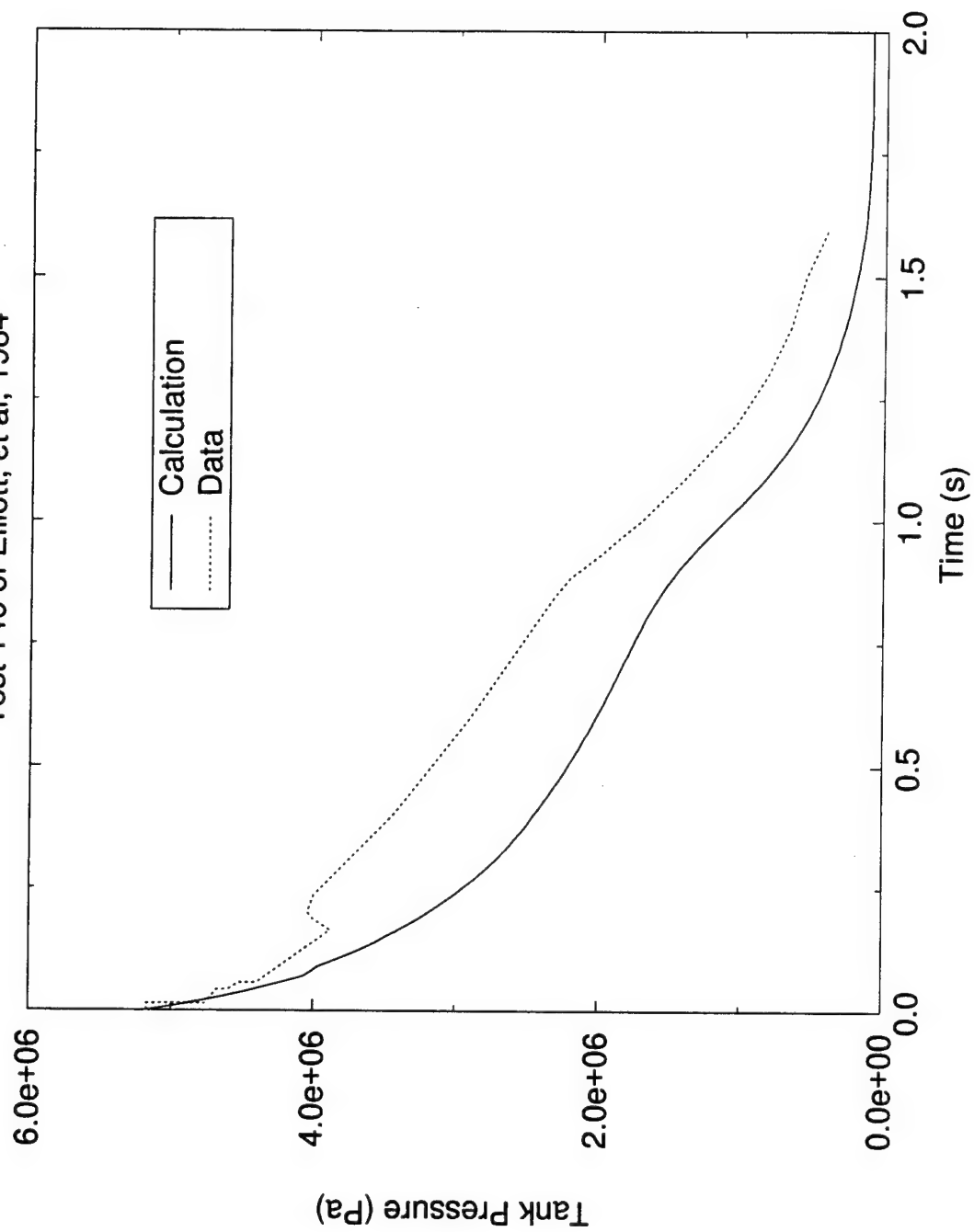
Figure 4.2 Comparison of Tank Pressure for Test 146 in Elliott et al, 1984
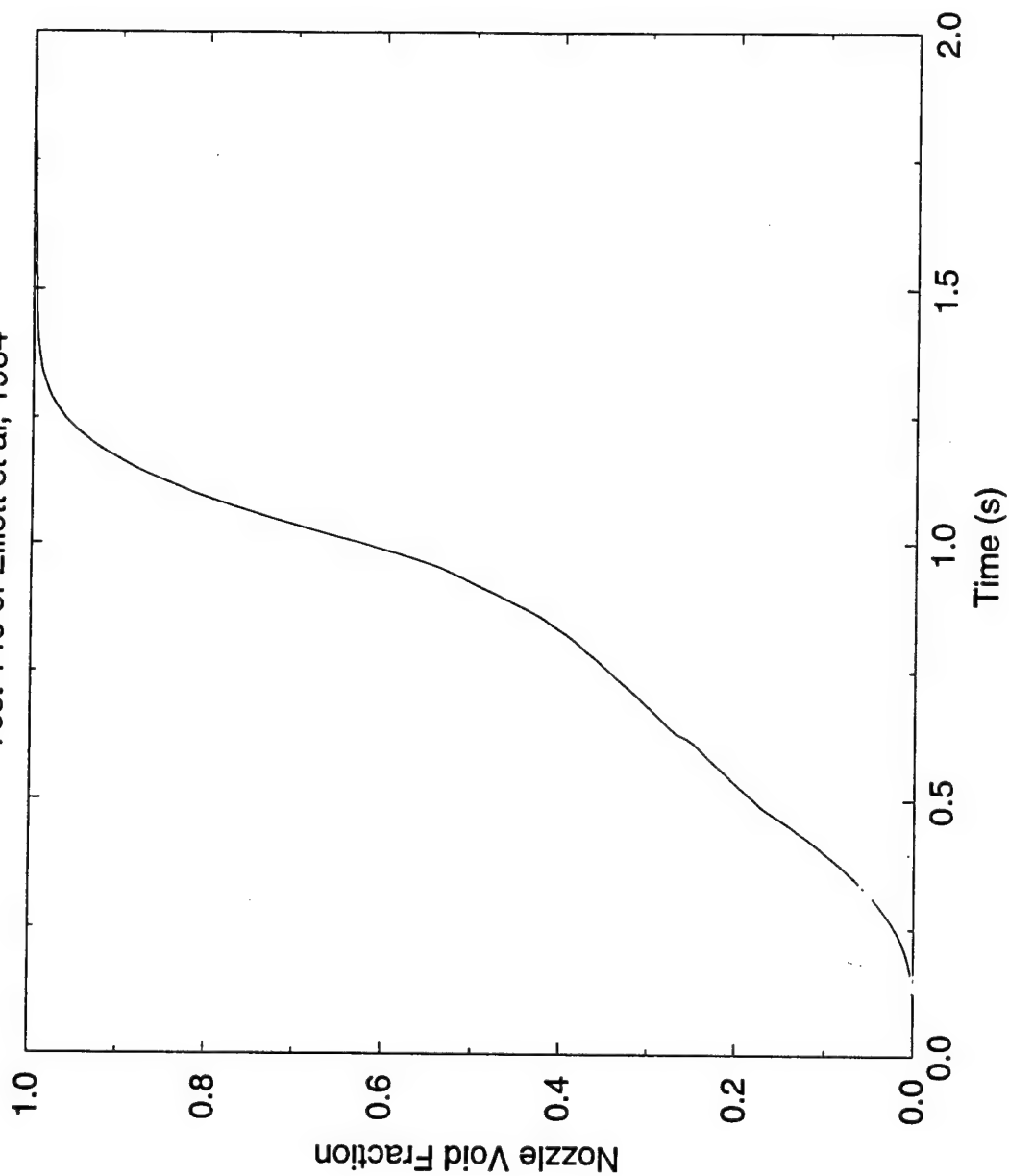
Figure 4.3 Variation of Nozzle Void Fraction with Time
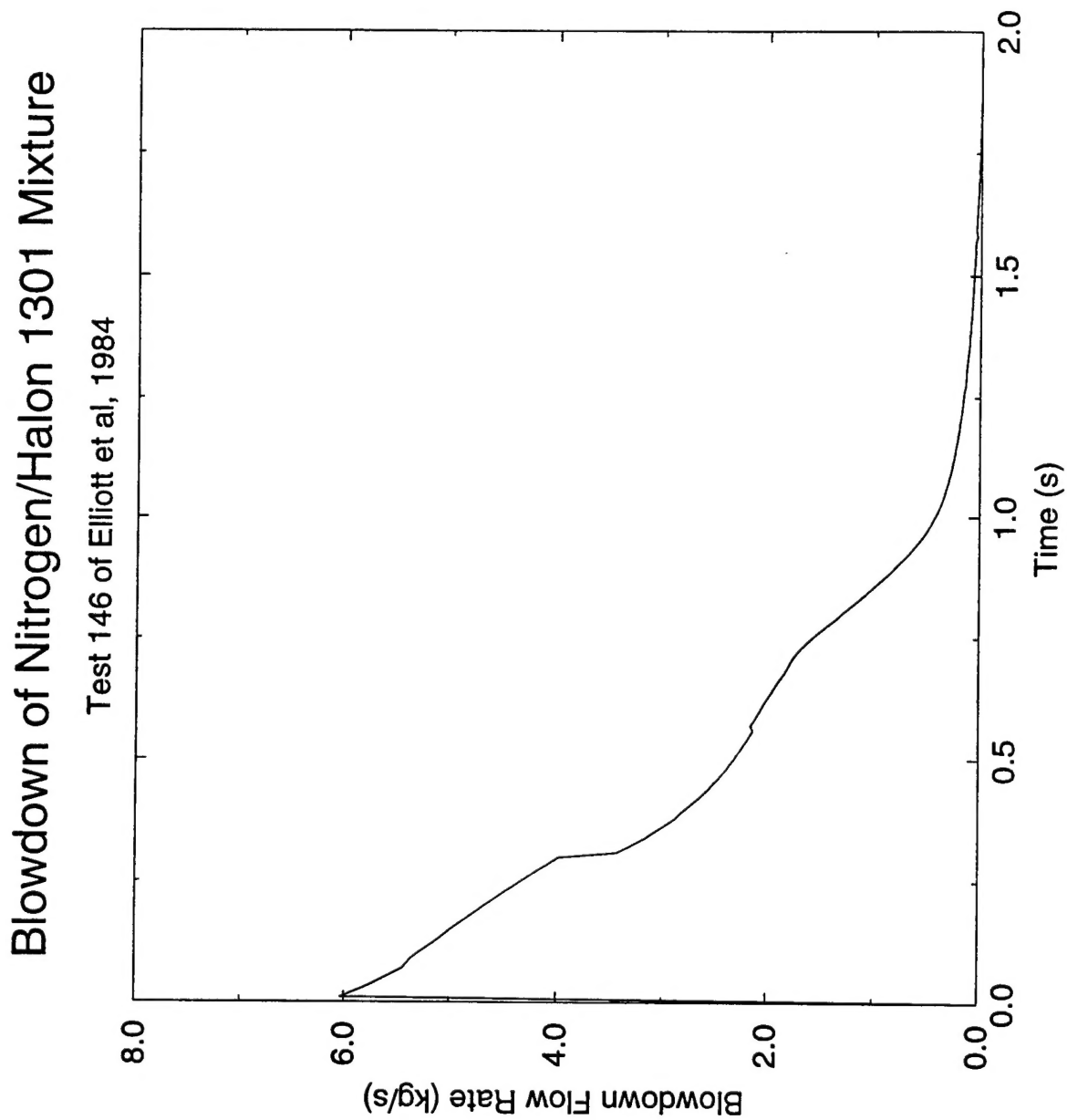
Figure 4.4: Variation of Discharge Flow Rate with Time
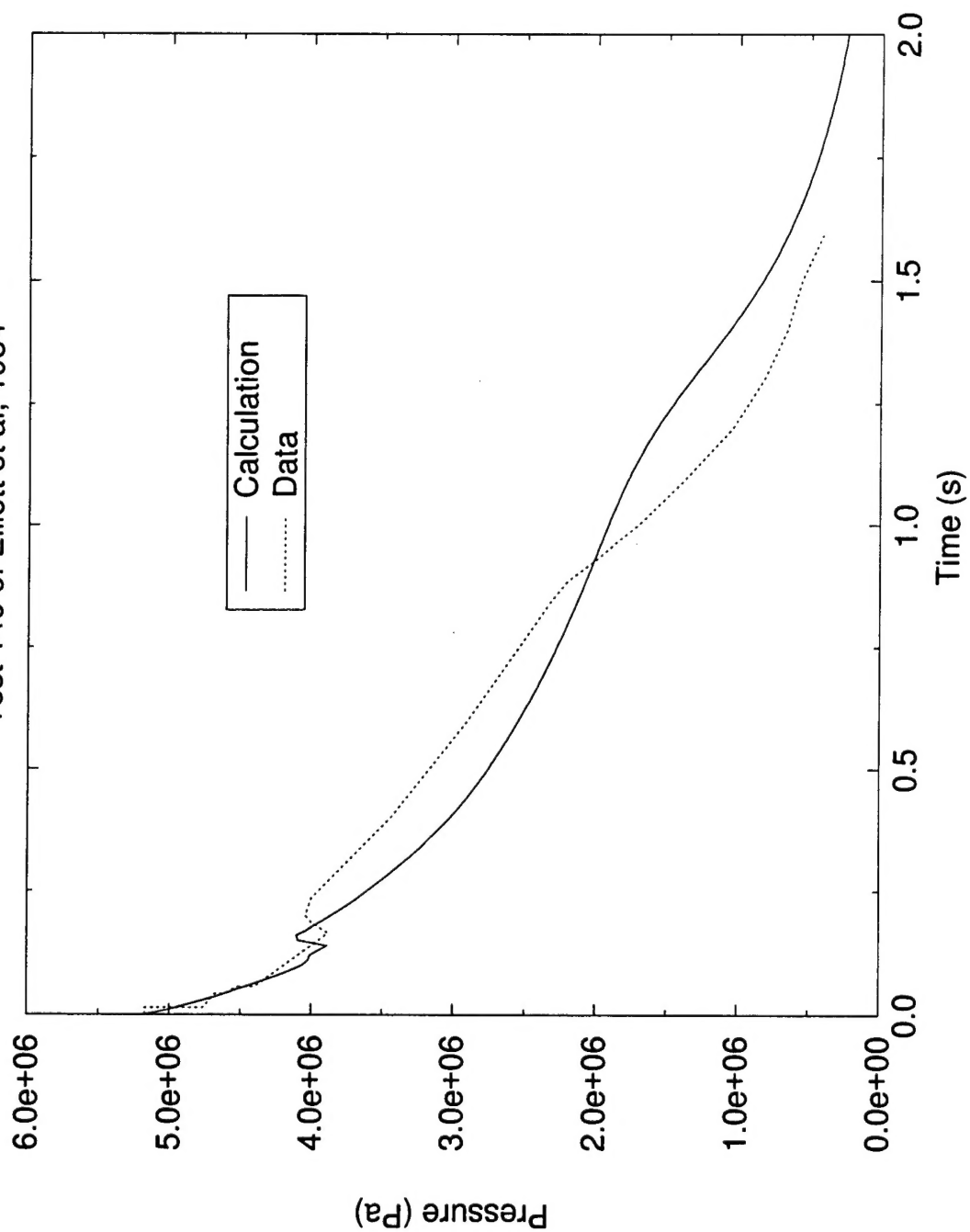
Figure 4.5: Effect of Nitrogen Release on Pressure Response
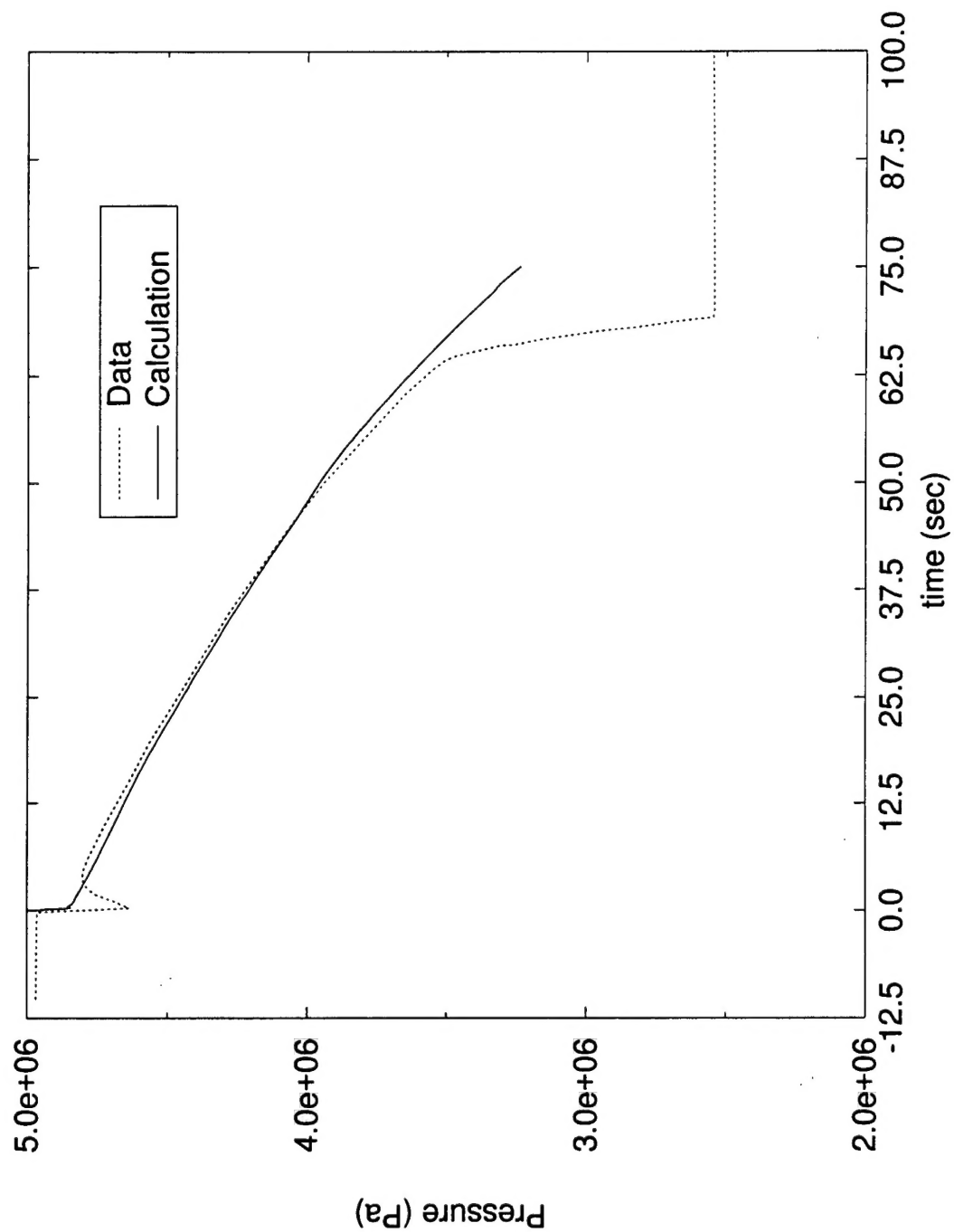
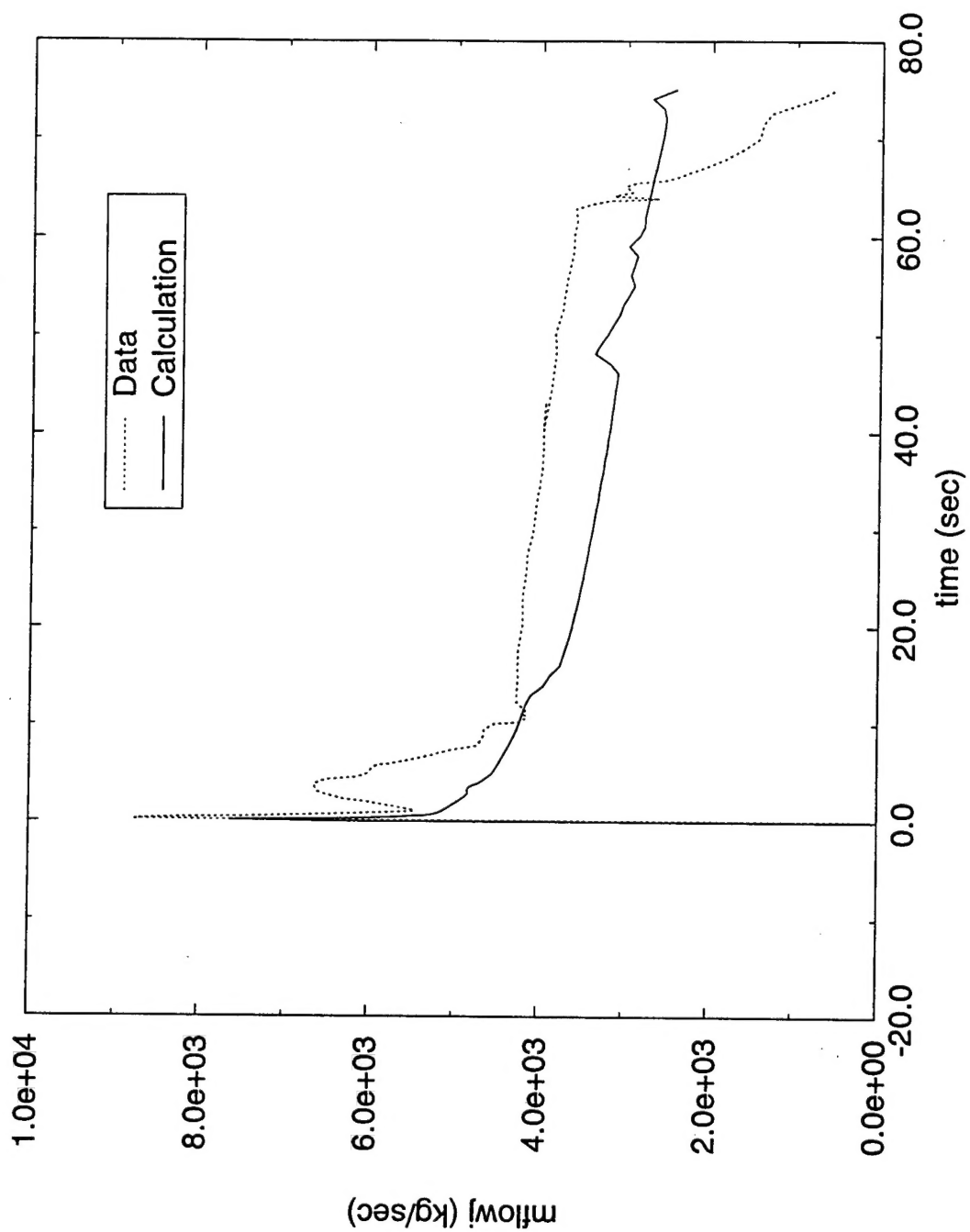Figure 4.6: Comparison of Vessel Pressure for Marviken Test No. 10

Figure 4.7: Comparison of Break Flow Rate for Marviken Test No. 10